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=> fil hcaplus
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FILE COVERS 1907 - 4 Aug 2006  VOL 145 ISS 7
FILE LAST UPDATED: 3 Aug 2006  (20060803/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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=> d stat que l21
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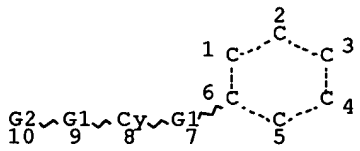

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

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L21 ANSWER 1 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:676948 HCAPLUS Full-text
TITLE: Lipoprotein nanoplatforms for diagnostic and therapeutic agents
INVENTOR(S): Zheng, Gang; Chance, Britton; Glickson, Jerry D.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006073419	A2	20060713	WO 2005-US11289	20050401

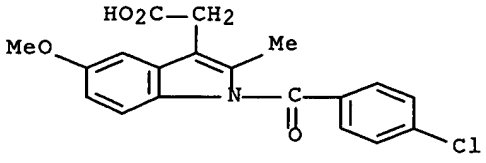
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-558502P P 20040401
US 2005-643825P P 20050114

AB The present invention provides a non-naturally occurring lipoprotein nanoplatform (LBNP) comprising at least one cell surface receptor ligand; at least one lipoprotein; and at least one diagnostic agent and/or at least one therapeutic agent. In embodiments of the present invention, the cell surface receptor ligand is not a low-d. lipoprotein receptor ligand and the cell surface receptor ligand is covalently bonded to the apoprotein. The present invention also provides pharmaceutical formulations comprising LBNPs and methods of making the LBNPs. Thus, low-d. lipoprotein (LDL) was reconstituted with photosensitizer pyropheophorbide cholesterol oleate (Pyro-CE). Pyro-CE was incorporated into LDL with a modest photosensitizer payload (Pyro-CE/LDL molar ratio < 50:1). The reconstitution efficiency of Pyro-CE-LDL was 45%. The reconstituted LDL-based photosensitizer was internalized exclusively by LDLR overexpressing human hepatoblastoma G2 (HepG2) tumor cells and accumulated in intracellular compartments such as endosomes or lysosomes. Destruction of tumor by using LDL receptor-targeted reconstituted Pyro-CE-LDL was also demonstrated.

IT 53-86-1, Indomethacin
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lipoprotein nanoplatforms comprising cell surface receptor ligand attached to apoprotein for diagnostic and therapeutic agents)

RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



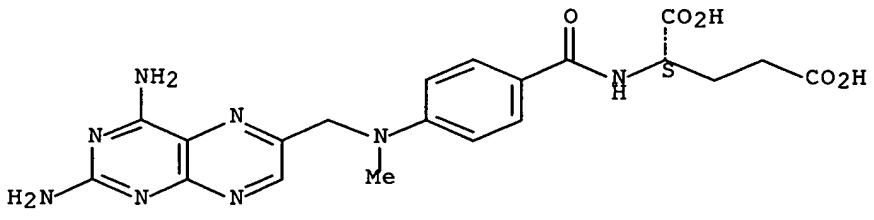
L21 ANSWER 2 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:433737 HCAPLUS Full-text
DOCUMENT NUMBER: 145:99018
TITLE: LGA-Dock/EM-Dock , Exploring Lamarckian genetic algorithms and energy-based local search for ligand-receptor docking
AUTHOR(S): Wiley, E. Ashley; MacDonald, Michael; Lambropoulos, Andreas; Harriman, D. Joseph; Deslongchamps, Ghislain
CORPORATE SOURCE: Department of Chemistry, St. Francis Xavier University, Antigonish, NS, B2G 2W5, Can.
SOURCE: Canadian Journal of Chemistry (2006), 84(3), 384-391
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors report the development of LGA-Dock and EM-Dock, two SVL-based docking programs for flexible ligand-rigid receptor docking applications. LGA-Dock is comprised of a stochastic population generator, a docking routine based on a Lamarckian genetic algorithm, and a local search function based on mol. mechanics (MM) energy minimization. Subsequent modifications of LGA-Dock to address performance issues produced EM-Dock, which proved to be as accurate and much faster than its predecessor despite the deletion of the genetic algorithm component. The basic performance of LGA-Dock and EM-Dock, compared with AutoDock and MOE 2004.03 docking routines is presented.

IT 59-05-2, Methotrexate
RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); BIOL (Biological study); PROC (Process)
(LGA-Dock/EM-Dock , exploring Lamarckian genetic algorithms and energy-based local search for flexible ligand- rigid receptor docking)

RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:97847 HCAPLUS Full-text
DOCUMENT NUMBER: 144:185209
TITLE: Screening ligands of nuclear receptors and their use for treatment of diseases
INVENTOR(S): Shiraki, Takuma; Kamiya, Shigetoshi; Jinkami, Hisato
PATENT ASSIGNEE(S): Biomolecular Engineering Research Institute, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 102 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

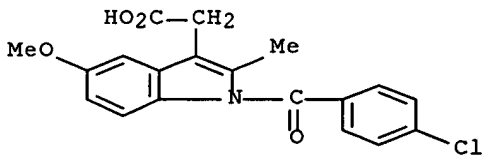
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006030037	A2	20060202	JP 2004-210868	20040716

PRIORITY APPLN. INFO.: JP 2004-210868 20040716
OTHER SOURCE(S): MARPAT 144:185209

AB This invention provides a process of screening of ligands of nuclear receptors such as PPARα. The ligands are specifically targeted the Cys with covalent binding or Arg and Tyr with hydrogen binding in the ligand binding domain of nuclear receptors. The ligands contain substitutable group RACHCH(CO)-RB-, RA(CO)-CHCHRB- (RA = hydrogen, univalent substitutable carboxyl, hydroxyl, amido, thiol group, RB = divalent hydrocarbon). The ligands can be displayed with formula R1CHCH(CO)R2R3 or R1(CO)CHCH-R2R3 (R1, R2 = hydrocarbon, R3 = univalent substitutable carboxyl, hydroxyl, amido, thiol group). The invention also provides protocol of theor. calcn. for prediction of three dimensional structure of receptor-ligand complex and detection of binding energy of ligands. The ligands provided in this invention can be used for treatment diseases.

IT 53-86-1, Indometacin
RL: BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(screening ligands of nuclear receptors and their use for treatment of diseases)

RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L21 ANSWER 4 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:15012 HCAPLUS Full-text
DOCUMENT NUMBER: 144:108223
TITLE: Preparation of cannabinoid receptor ligands
INVENTOR(S): Shankar, Bandarpalle B.; Gilbert, Eric; Rizvi, Razia K.; Huang, Chunli; Kozlowski, Joseph A.; McCombie, Stuart; Shih, Neng-Yang
PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006002133	A1	20060105	WO 2005-US21870	20050621
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2006100228	A1	20060511	US 2005-157510	20050621

PRIORITY APPLN. INFO.: US 2004-581837P P 20040622
OTHER SOURCE(S): MARPAT 144:108223
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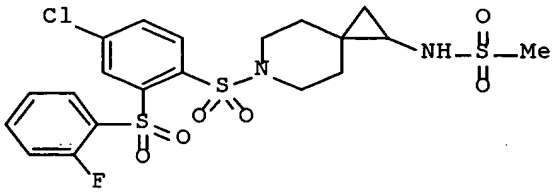

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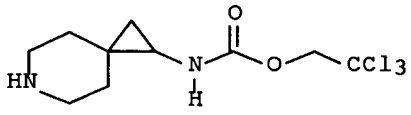

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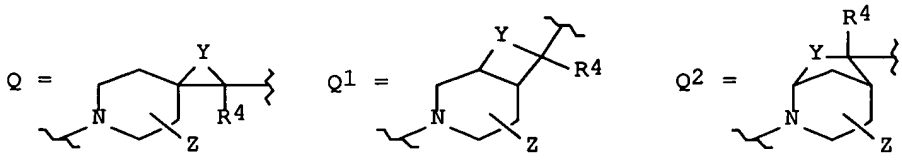


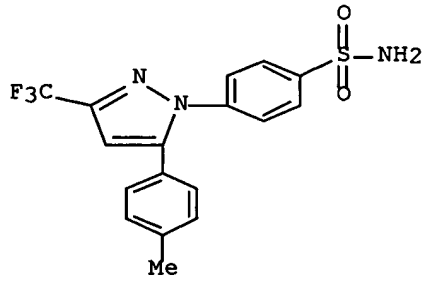
AB Compds. of formula R1-L1-A(Xm)-L2-B-N(R5)-L3-R6 [R1 = H, alkyl, CF3, etc.; R5, R6 = H, alkyl, haloalkyl, aryl, heterocycloalkyl, heteroaryl; A = Ph, naphthyl, pyridyl, thiazolyl, etc.; B = Q, Q1, Q2, etc., R4 = H, alkyl; Y = (C(R7)2)p, O(C(R7)2)q, S(O2)(C(R7)2)r, etc., R7 = H, alkyl, heteroaryl, cycloalkyl, etc., p = 1-3, q = 1, 2; Z = (R2)n, R2 = H, OH, halo, alkoxy, cycloalkyl, etc., n = 0-4; L1 = (C(R7)2)p, CO, SO, etc.; L2 = (C(R7)2)p, CO2, CF2, etc.; L3 = C(R7)2, CO, O, etc.] were prepared For example, spiro-

piperidine I was prepared in several steps from amine II. These compds. can exhibit anti-inflammatory and immunomodulatory activity, and can be effective as CB2 receptor ligands in treating cancer and inflammatory, immunomodulatory or respiratory diseases or conditions.

IT 169590-42-5, Celecoxib
RL: PAC (Pharmacological activity); BIOL (Biological study)
(co-administered agent; preparation of piperidine derivs. as cannabinoid receptor ligands co-administered with celecoxib)

RN 169590-42-5 HCAPLUS

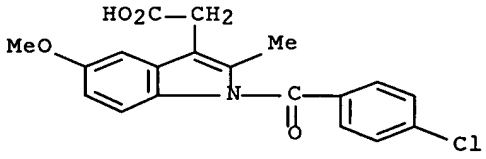
CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



IT 53-86-1, Indomethacin
RL: PAC (Pharmacological activity); BIOL (Biological study)
(co-administered agent; preparation of piperidine derivs. as cannabinoid receptor ligands co-administered with indomethacin)

RN 53-86-1 HCAPLUS

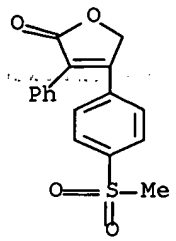
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



IT 162011-90-7, Rofecoxib
RL: PAC (Pharmacological activity); BIOL (Biological study)
(co-administered agent; preparation of piperidine derivs. as cannabinoid receptor ligands co-administered with rofecoxib)

RN 162011-90-7 HCAPLUS

CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



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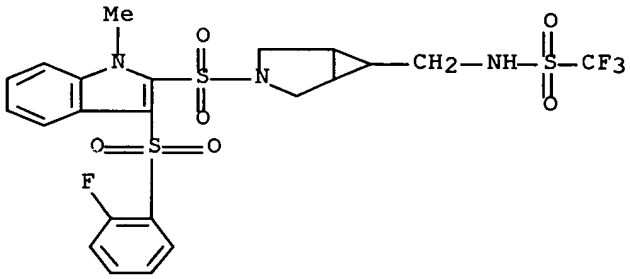
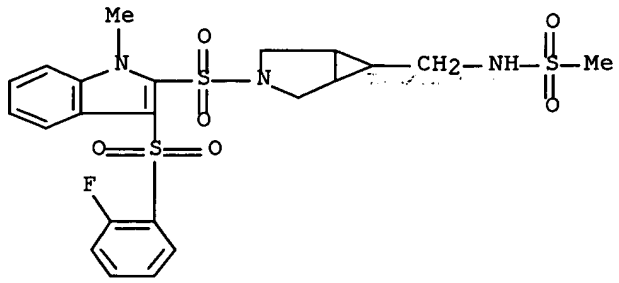
872982-99-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperidine derivs. as cannabinoid receptor ligands)

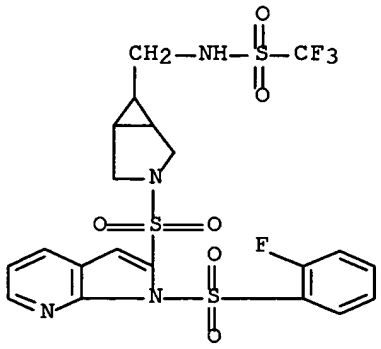
RN 872982-29-1 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[[3-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



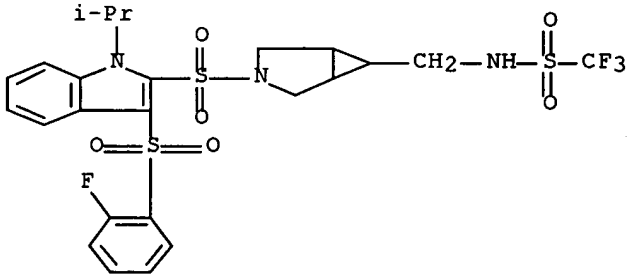
RN 872982-31-5 HCAPLUS
CN Methanesulfonamide, N-[[3-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



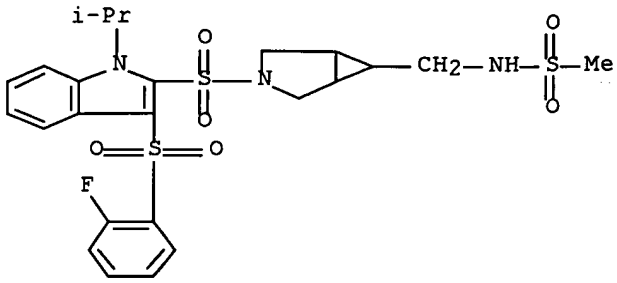
RN 872982-33-7 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[[3-[[1-[(2-fluorophenyl)sulfonyl]-1H-pyrrolo[2,3-b]pyridin-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



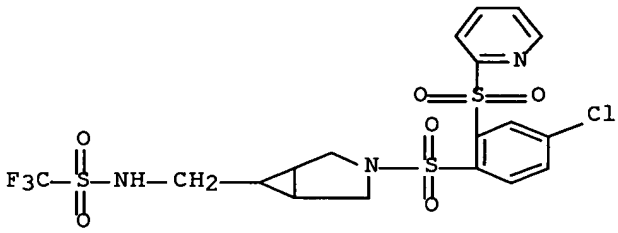
RN 872982-34-8 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[[3-[[3-[(2-fluorophenyl)sulfonyl]-1-(1-methylethyl)-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



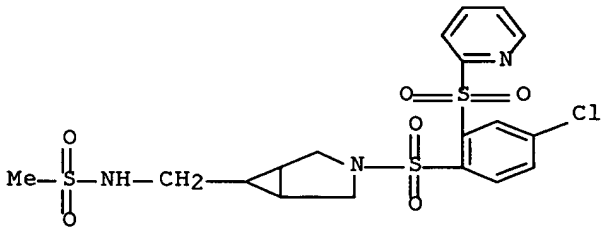
RN 872982-35-9 HCAPLUS
CN Methanesulfonamide, N-[[3-[[3-[(2-fluorophenyl)sulfonyl]-1-(1-methylethyl)-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



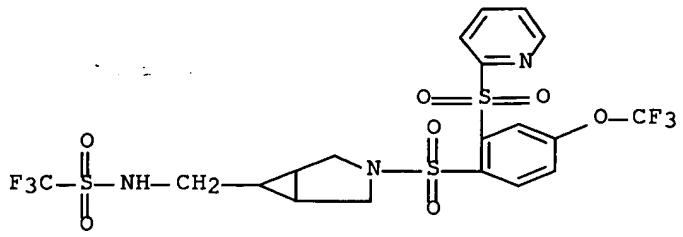
RN 872982-36-0 HCAPLUS
CN Methanesulfonamide, N-[[3-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



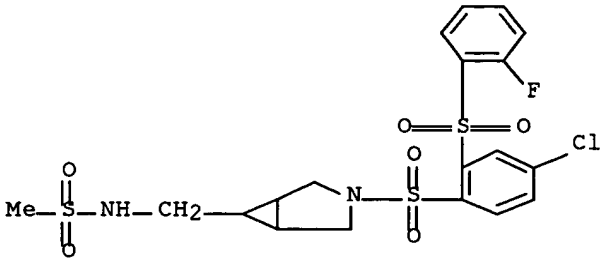
RN 872982-37-1 HCAPLUS
CN Methanesulfonamide, N-[[3-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



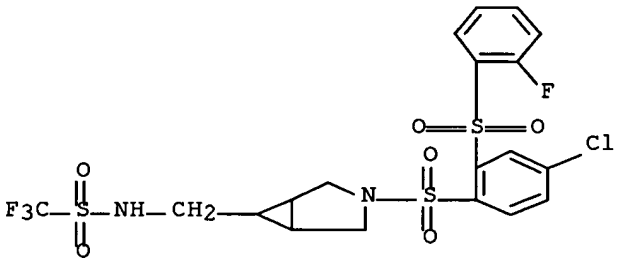
RN 872982-38-2 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[[3-[[2-(2-pyridinylsulfonyl)-4-(trifluoromethoxy)phenyl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



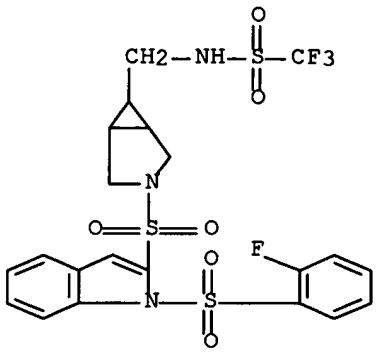
RN 872982-39-3 HCAPLUS
CN Methanesulfonamide, N-[[3-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



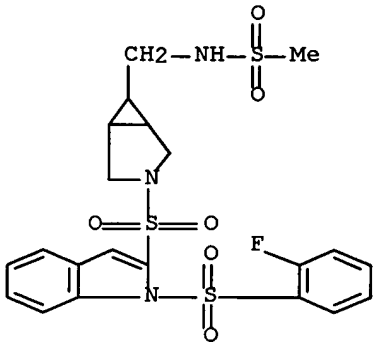
RN 872982-41-7 HCAPLUS
CN Methanesulfonamide, N-[[3-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



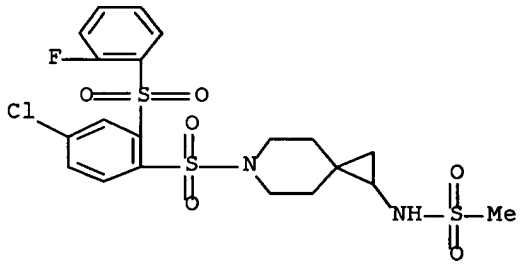
RN 872982-42-8 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[[3-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)



RN 872982-43-9 HCAPLUS
CN Methanesulfonamide, N-[[3-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]- (9CI) (CA INDEX NAME)

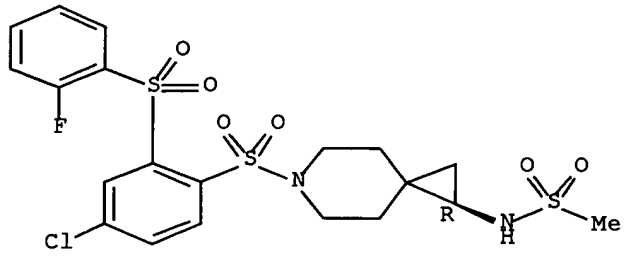


RN 872982-46-2 HCAPLUS
CN Methanesulfonamide, N-[6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



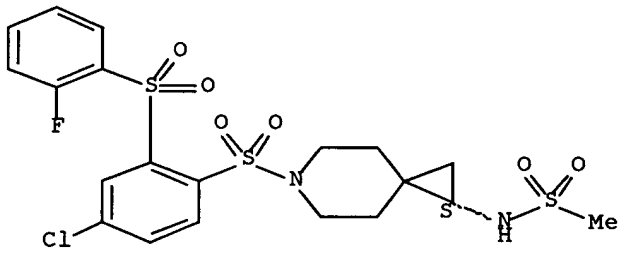
RN 872982-47-3 HCAPLUS
CN Methanesulfonamide, N-[(1R)-6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



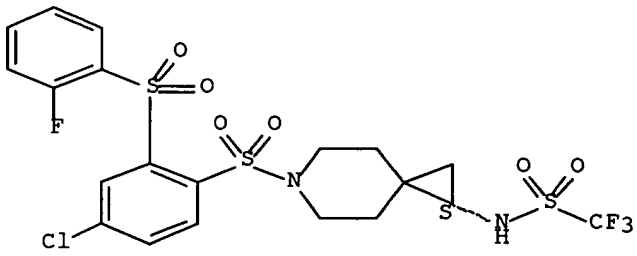
RN 872982-48-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

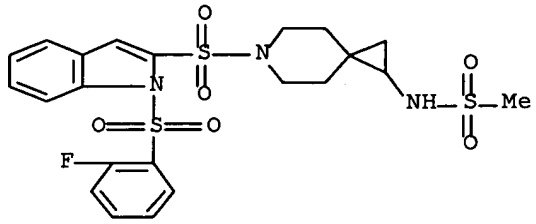


RN 872982-49-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

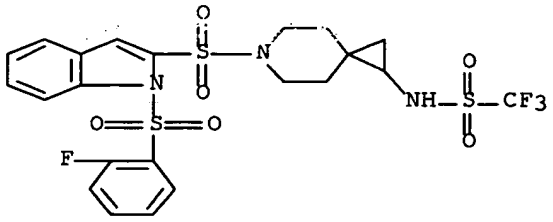
Absolute stereochemistry.



RN 872982-50-8 HCAPLUS
CN Methanesulfonamide, N-[6-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)

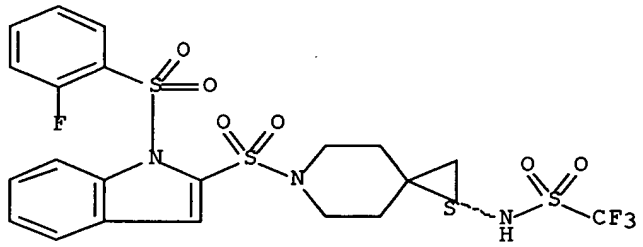


RN 872982-51-9 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)

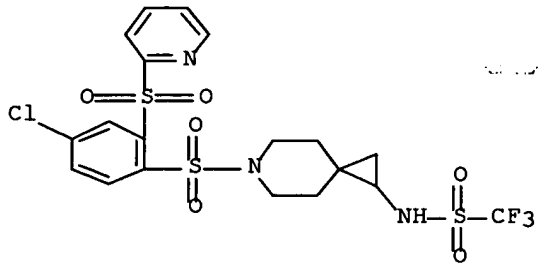


RN 872982-52-0 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-6-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)

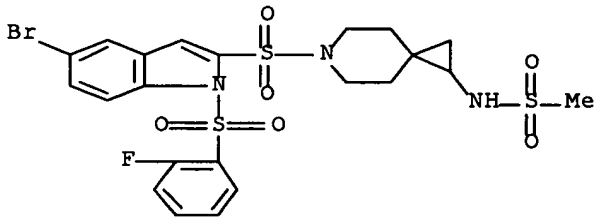
Absolute stereochemistry.



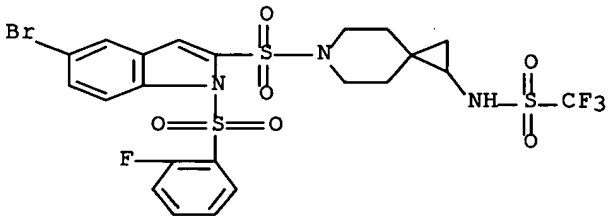
RN 872982-53-1 HCAPLUS
CN Methanesulfonamide, N-[6-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



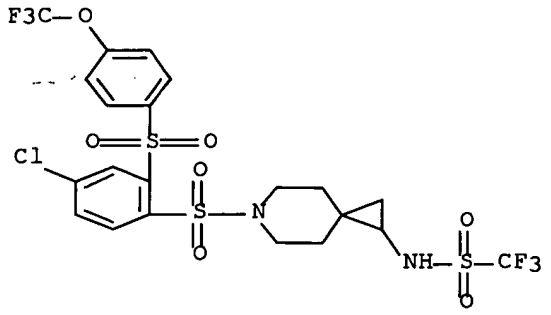
RN 872982-54-2 HCAPLUS
CN Methanesulfonamide, N-[6-[[5-bromo-1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



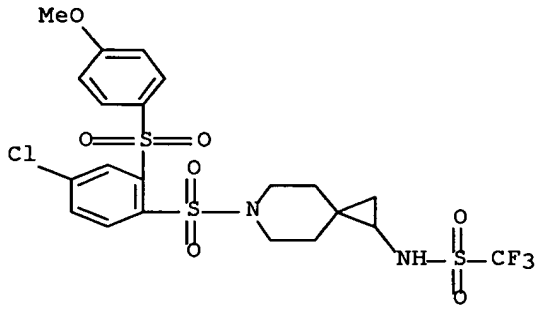
RN 872982-55-3 HCAPLUS
CN Methanesulfonamide, N-[6-[[5-bromo-1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



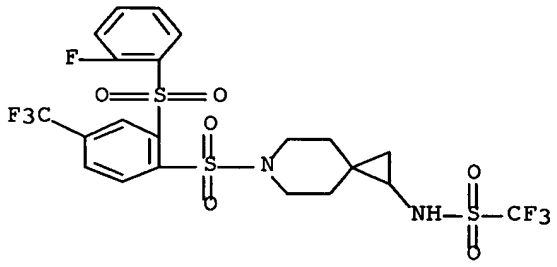
RN 872982-56-4 HCAPLUS
CN Methanesulfonamide, N-[6-[[4-chloro-2-[[4-(trifluoromethoxy)phenyl]sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



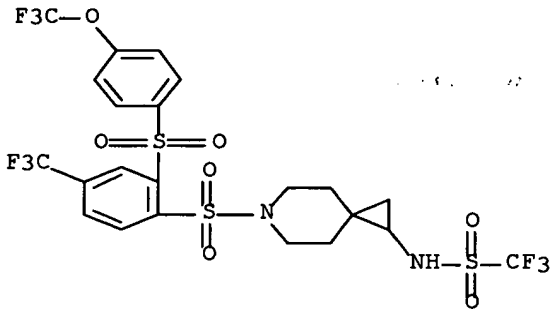
RN 872982-57-5 HCAPLUS
CN Methanesulfonamide, N-[6-[[4-chloro-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



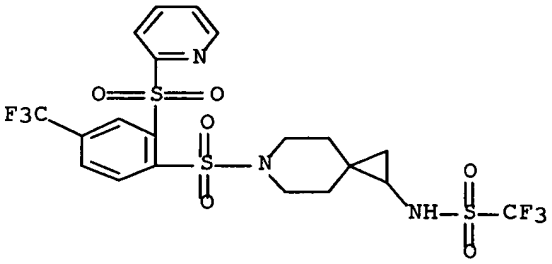
RN 872982-58-6 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



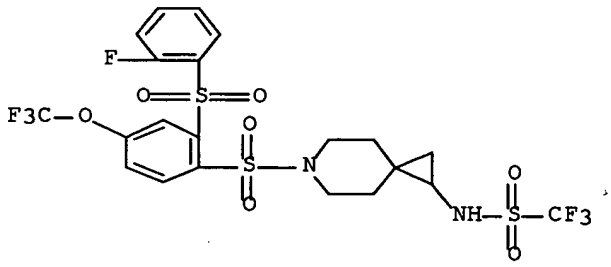
RN 872982-59-7 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[2-[[4-(trifluoromethoxy)phenyl]sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



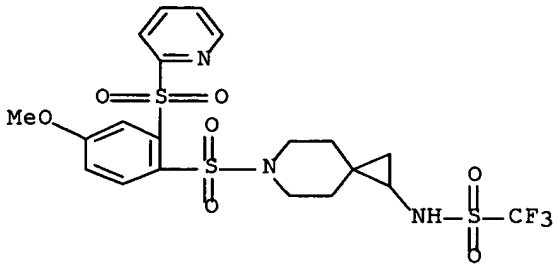
RN 872982-60-0 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[2-(2-pyridinylsulfonyl)-4-(trifluoromethyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



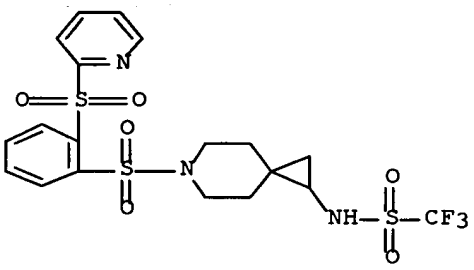
RN 872982-61-1 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



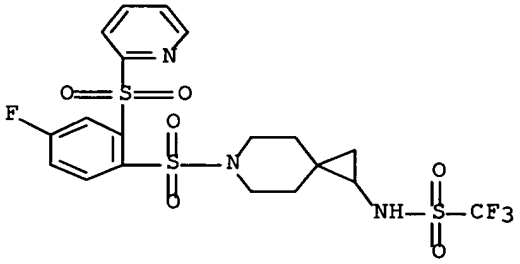
RN 872982-62-2 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[4-methoxy-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



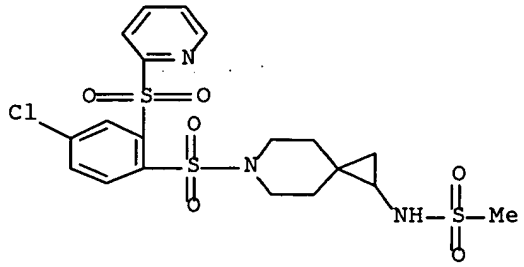
RN 872982-63-3 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



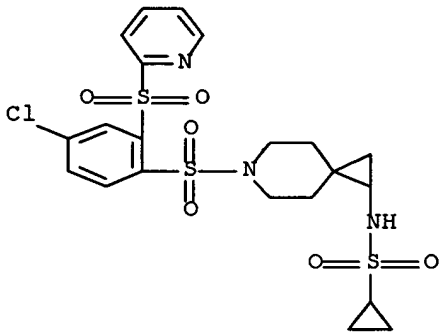
RN 872982-64-4 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[4-fluoro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



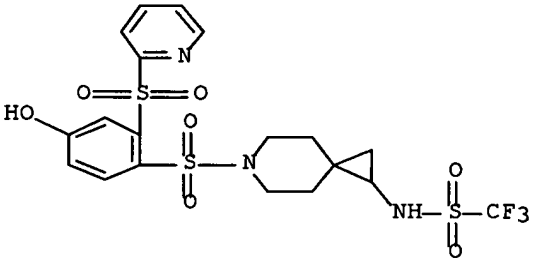
RN 872982-65-5 HCAPLUS
CN Methanesulfonamide, N-[6-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



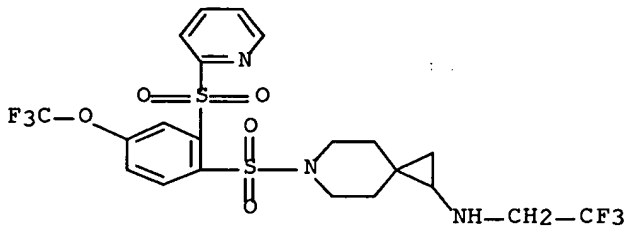
RN 872982-66-6 HCAPLUS
CN Cyclopropanesulfonamide, N-[6-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



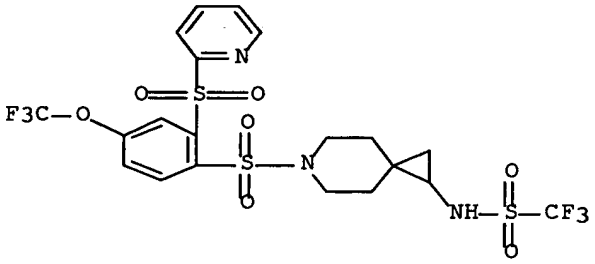
RN 872982-67-7 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[4-hydroxy-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



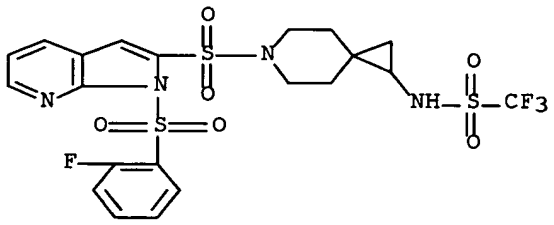
RN 872982-68-8 HCAPLUS
CN 6-Azaspiro[2.5]octan-1-amine, 6-[[2-(2-pyridinylsulfonyl)-4-(trifluoromethoxy)phenyl]sulfonyl]-N-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)



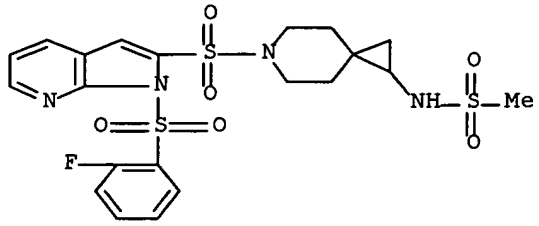
RN 872982-69-9 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[2-(2-pyridinylsulfonyl)-4-(trifluoromethoxy)phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



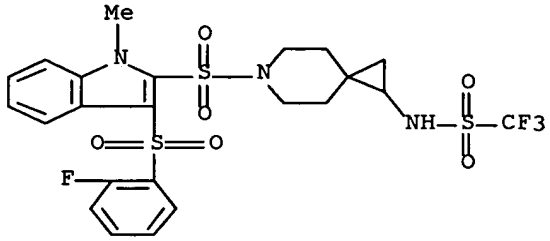
RN 872982-71-3 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[1-[(2-fluorophenyl)sulfonyl]-1H-pyrrolo[2,3-b]pyridin-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



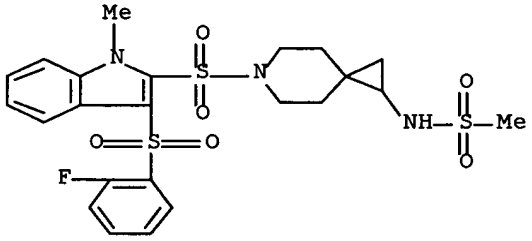
RN 872982-72-4 HCAPLUS
CN Methanesulfonamide, N-[6-[[1-[(2-fluorophenyl)sulfonyl]-1H-pyrrolo[2,3-b]pyridin-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



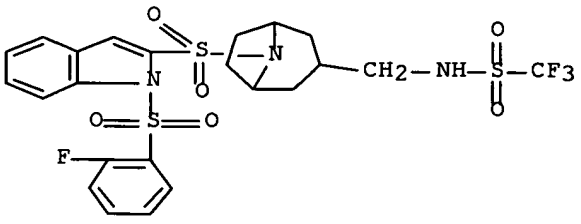
RN 872982-73-5 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[6-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



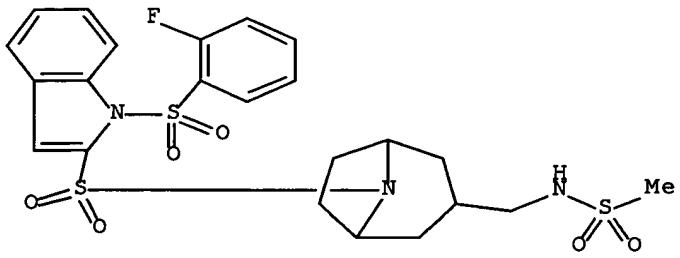
RN 872982-74-6 HCAPLUS
CN Methanesulfonamide, N-[6-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)



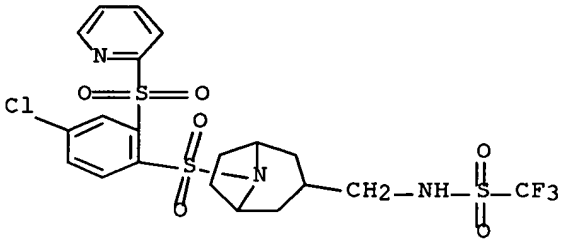
RN 872982-75-7 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[[8-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-8-azabicyclo[3.2.1]oct-3-yl]methyl]- (9CI) (CA INDEX NAME)



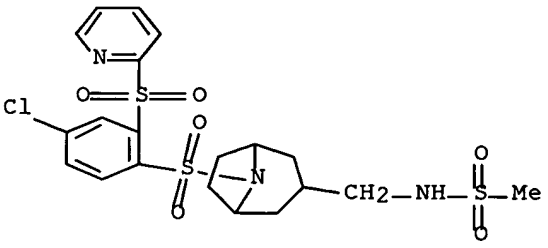
RN 872982-76-8 HCAPLUS
CN Methanesulfonamide, N-[[8-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-8-azabicyclo[3.2.1]oct-3-yl]methyl]- (9CI) (CA INDEX NAME)



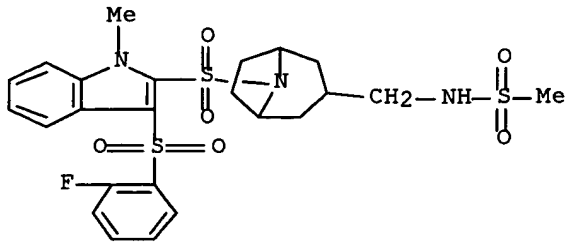
RN 872982-79-1 HCAPLUS
CN Methanesulfonamide, N-[[8-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-8-azabicyclo[3.2.1]oct-3-yl]methyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



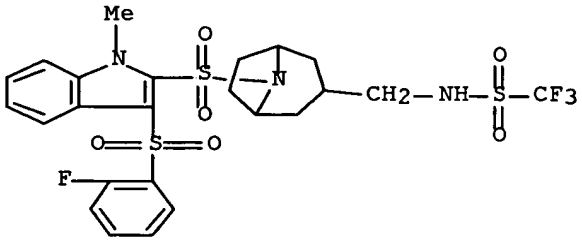
RN 872982-80-4 HCAPLUS
CN Methanesulfonamide, N-[[8-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-8-azabicyclo[3.2.1]oct-3-yl]methyl]- (9CI) (CA INDEX NAME)



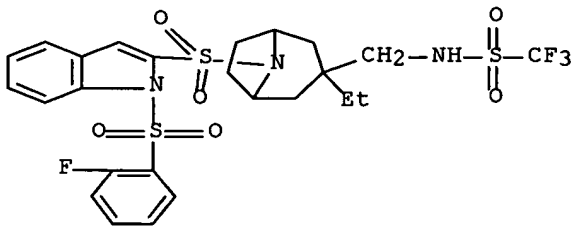
RN 872982-81-5 HCAPLUS
CN Methanesulfonamide, N-[[8-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]-8-azabicyclo[3.2.1]oct-3-yl]methyl]- (9CI) (CA INDEX NAME)



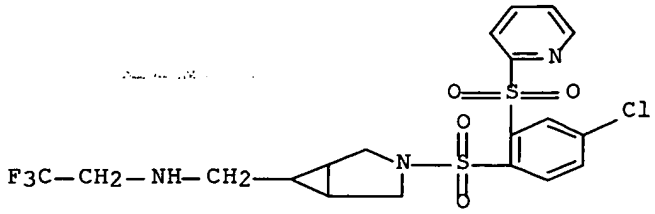
RN 872982-82-6 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[[8-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]-8-azabicyclo[3.2.1]oct-3-yl]methyl]- (9CI) (CA INDEX NAME)



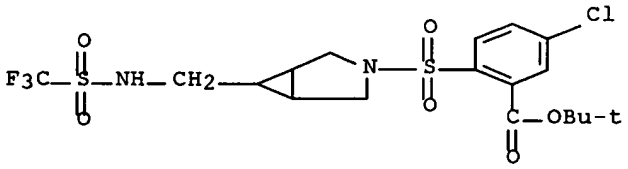
RN 872982-83-7 HCAPLUS
CN Methanesulfonamide, N-[[3-ethyl-8-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-8-azabicyclo[3.2.1]oct-3-yl]methyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



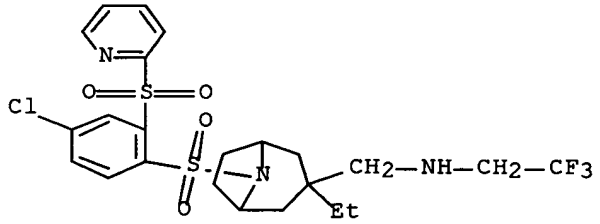
RN 872982-85-9 HCAPLUS
CN 3-Azabicyclo[3.1.0]hexane-6-methanamine, 3-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-N-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)



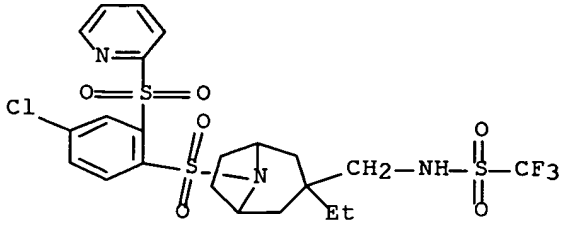
RN 872982-86-0 HCAPLUS
CN Benzoic acid, 5-chloro-2-[[6-[[[(trifluoromethyl)sulfonyl]amino]methyl]-3-azabicyclo[3.1.0]hex-3-yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



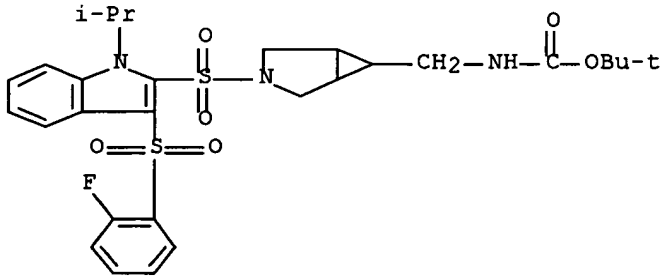
RN 872982-87-1 HCAPLUS
CN 8-Azabicyclo[3.2.1]octane-3-methanamine, 8-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-3-ethyl-N-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)



RN 872982-89-3 HCAPLUS
CN Methanesulfonamide, N-[[8-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-3-ethyl-8-azabicyclo[3.2.1]oct-3-yl]methyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

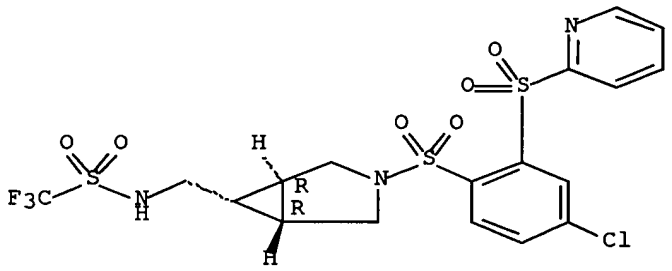


RN 872982-91-7 HCAPLUS
CN Carbamic acid, [[3-[[3-[(2-fluorophenyl)sulfonyl]-1-(1-methylethyl)-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



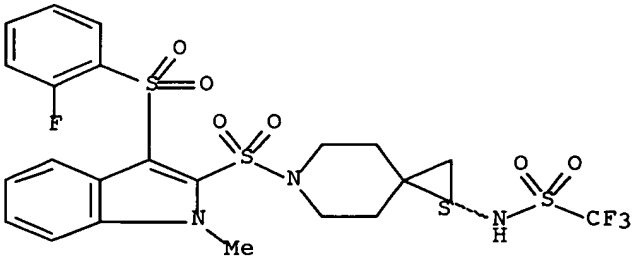
RN 872982-95-1 HCAPLUS
CN Methanesulfonamide, N-[[(1R,5R)-3-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



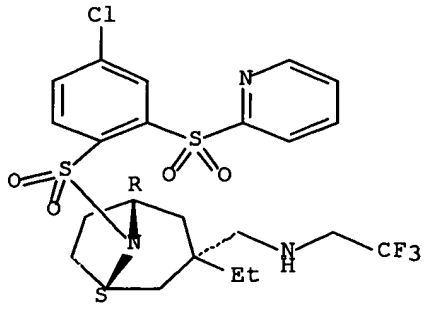
RN 872982-97-3 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-6-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



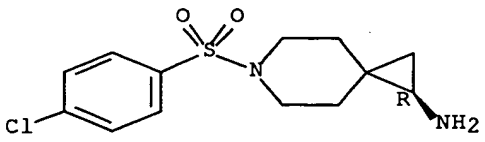
RN 872982-99-5 HCAPLUS
CN 8-Azabicyclo[3.2.1]octane-3-methanamine, 8-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-3-ethyl-N-(2,2,2-trifluoroethyl)-, (3-endo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



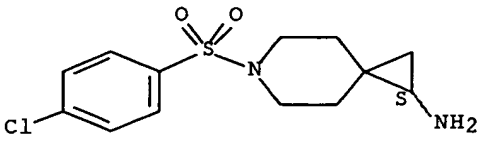
IT 872983-30-7P 872983-32-9P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperidine derivs. as cannabinoid receptor ligands)
RN 872983-30-7 HCAPLUS
CN 6-Azaspiro[2.5]octan-1-amine, 6-[(4-chlorophenyl)sulfonyl]-, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



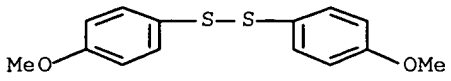
RN 872983-32-9 HCAPLUS
CN 6-Azaspiro[2.5]octan-1-amine, 6-[(4-chlorophenyl)sulfonyl]-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

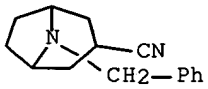


IT 5335-87-5, 4-Methoxyphenyl disulfide 185985-38-0
871727-08-1 872983-18-1 872983-50-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of piperidine derivs. as cannabinoid receptor

ligands)
RN 5335-87-5 HCAPLUS
CN Disulfide, bis(4-methoxyphenyl) (9CI) (CA INDEX NAME)

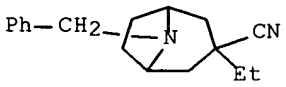


RN 185985-38-0 HCAPLUS
CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 8-(phenylmethyl)- (9CI) (CA INDEX NAME)

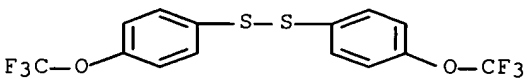


RN 871727-08-1 HCAPLUS
CN 3-Azabicyclo[3.1.0]hexane-6-methanol, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 872983-18-1 HCAPLUS
CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 3-ethyl-8-(phenylmethyl)- (9CI) (CA INDEX NAME)



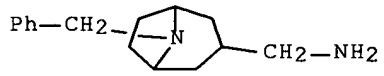
RN 872983-50-1 HCAPLUS
CN Disulfide, bis[4-(trifluoromethoxy)phenyl] (9CI) (CA INDEX NAME)



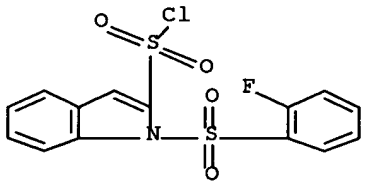
IT 223570-84-1P 530116-15-5P 871727-09-2P
871727-10-5P 871727-11-6P 871727-13-8P
872983-20-5P 872983-21-6P 872983-23-8P
872983-28-3P 872983-34-1P 872983-36-3P
872983-38-5P 872983-40-9P 872983-42-1P

872983-44-3P 872983-46-5P 872983-48-7P
872983-52-3P 872983-59-0P 872983-61-4P
872983-65-8P 872983-67-0P 872983-69-2P
872983-71-6P 872983-73-8P 872983-83-0P
872983-88-5P 872983-90-9P 872983-92-1P
872983-94-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperidine derivs. as cannabinoid receptor ligands)

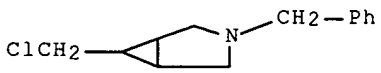
RN 223570-84-1 HCAPLUS
CN 8-Azabicyclo[3.2.1]octane-3-methanamine, 8-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 530116-15-5 HCAPLUS
CN 1H-Indole-2-sulfonyl chloride, 1-[(2-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

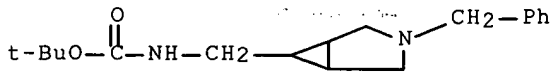


RN 871727-09-2 HCAPLUS
CN 3-Azabicyclo[3.1.0]hexane, 6-(chloromethyl)-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

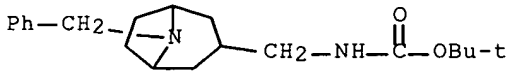


RN 871727-10-5 HCAPLUS
CN 3-Azabicyclo[3.1.0]hexane, 6-(azidomethyl)-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

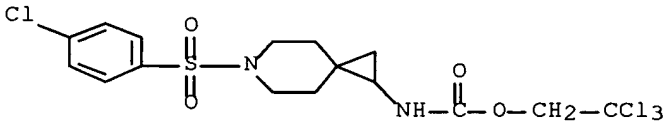
RN 871727-11-6 HCAPLUS
CN Carbamic acid, [[3-(phenylmethyl)-3-azabicyclo[3.1.0]hex-6-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



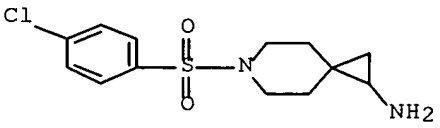
RN 871727-13-8 HCAPLUS
CN Carbamic acid, [[8-(phenylmethyl)-8-azabicyclo[3.2.1]oct-3-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



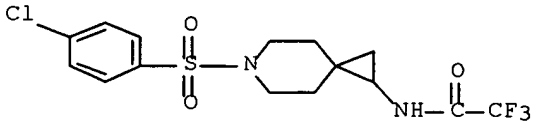
RN 872983-20-5 HCAPLUS
CN Carbamic acid, [6-[(4-chlorophenyl)sulfonyl]-6-azaspiro[2.5]oct-1-yl]-, 2,2,2-trichloroethyl ester (9CI) (CA INDEX NAME)



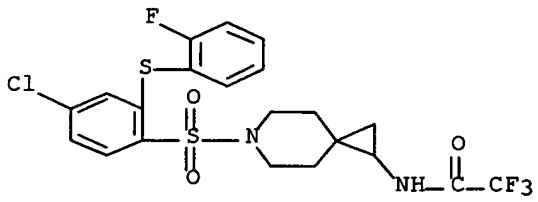
RN 872983-21-6 HCAPLUS
CN 6-Azaspiro[2.5]octan-1-amine, 6-[(4-chlorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 872983-23-8 HCAPLUS
CN Acetamide, N-[6-[(4-chlorophenyl)sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

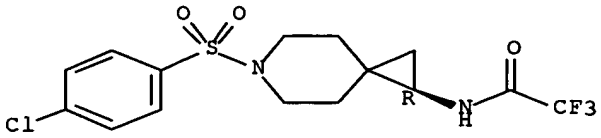


RN 872983-28-3 HCAPLUS
CN Acetamide, N-[6-[[4-chloro-2-[(2-fluorophenyl)thio]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)



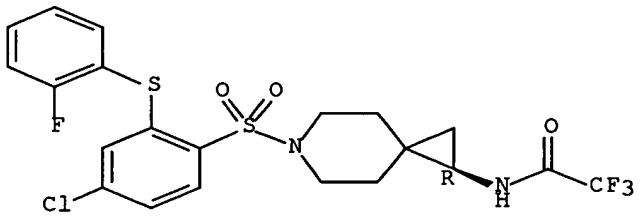
RN 872983-34-1 HCAPLUS
CN Acetamide, N-[(1R)-6-[(4-chlorophenyl)sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



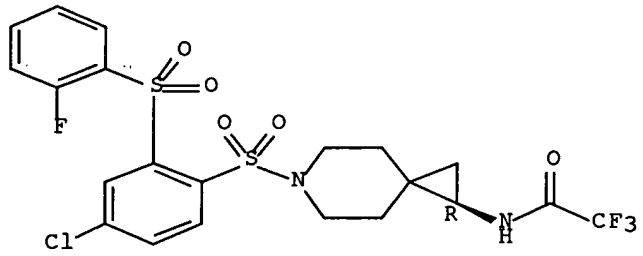
RN 872983-36-3 HCAPLUS
CN Acetamide, N-[(1R)-6-[[4-chloro-2-[(2-fluorophenyl)thio]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



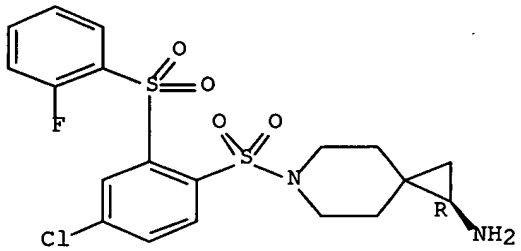
RN 872983-38-5 HCAPLUS
CN Acetamide, N-[(1R)-6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



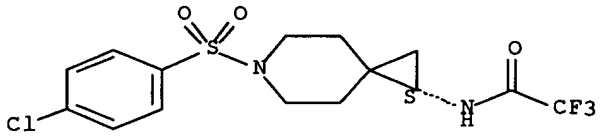
RN 872983-40-9 HCAPLUS
CN 6-Azaspiro[2.5]octan-1-amine, 6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



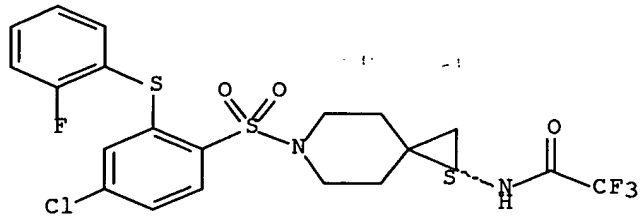
RN 872983-42-1 HCAPLUS
CN Acetamide, N-[(1S)-6-[(4-chlorophenyl)sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



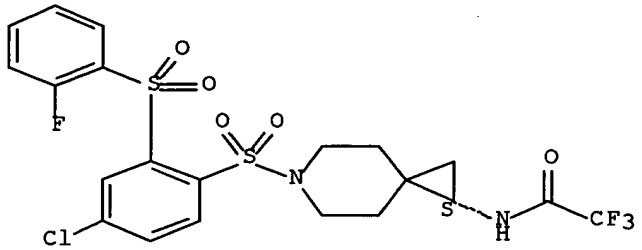
RN 872983-44-3 HCAPLUS
CN Acetamide, N-[(1S)-6-[[4-chloro-2-[(2-fluorophenyl)thio]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



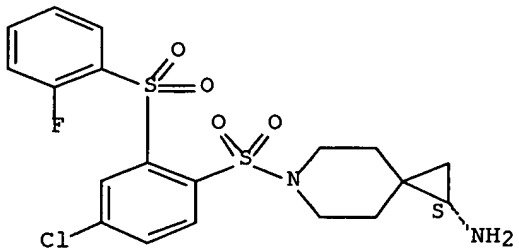
RN 872983-46-5 HCAPLUS
CN Acetamide, N-[(1S)-6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



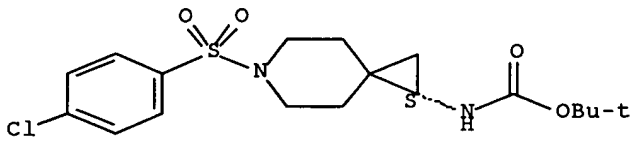
RN 872983-48-7 HCAPLUS
CN 6-Azaspiro[2.5]octan-1-amine, 6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



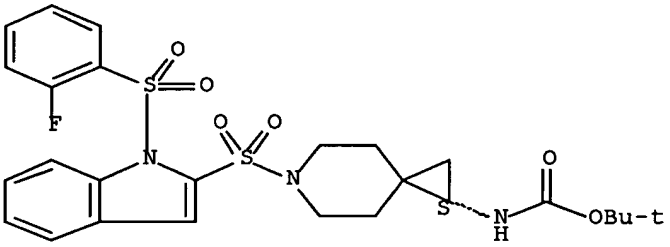
RN 872983-52-3 HCAPLUS
CN Carbamic acid, [(1S)-6-[(4-chlorophenyl)sulfonyl]-6-azaspiro[2.5]oct-1-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



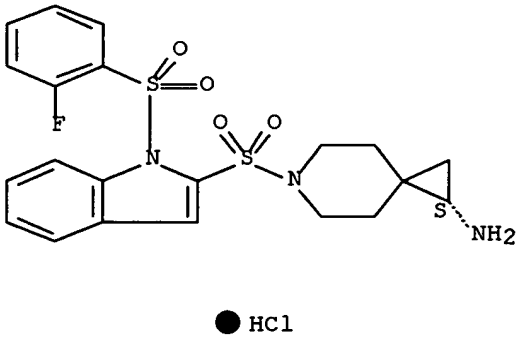
RN 872983-59-0 HCAPLUS
CN Carbamic acid, [(1S)-6-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

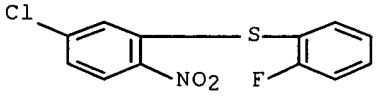


RN 872983-61-4 HCAPLUS
CN 6-Azaspiro[2.5]octan-1-amine, 6-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-, monohydrochloride, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

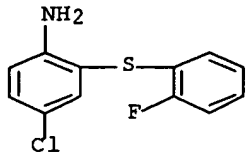


RN 872983-65-8 HCAPLUS
CN Benzene, 4-chloro-2-[(2-fluorophenyl)thio]-1-nitro- (9CI) (CA INDEX NAME)



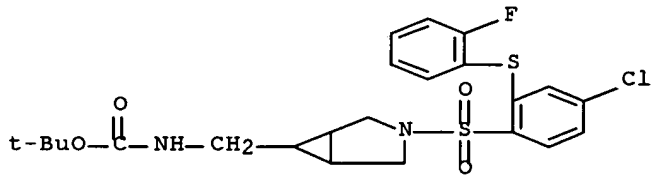
RN 872983-67-0 HCAPLUS

CN Benzenamine, 4-chloro-2-[(2-fluorophenyl)thio]- (9CI) (CA INDEX NAME)



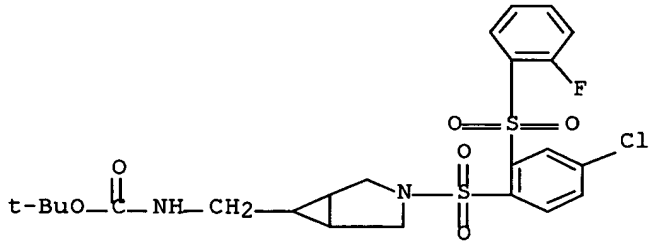
RN 872983-69-2 HCAPLUS

CN Carbamic acid, [[3-[[4-chloro-2-[(2-fluorophenyl)thio]phenyl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



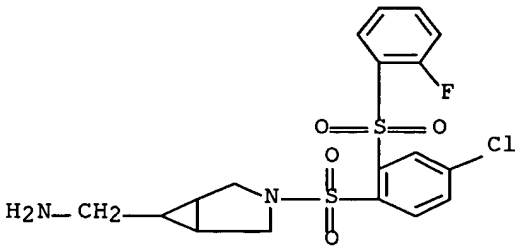
RN 872983-71-6 HCAPLUS

CN Carbamic acid, [[3-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

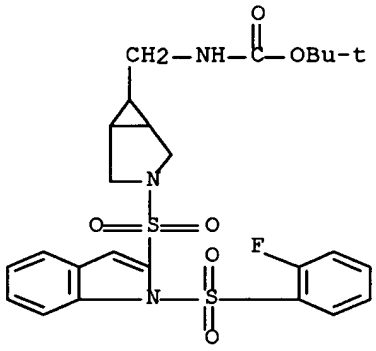


RN 872983-73-8 HCAPLUS

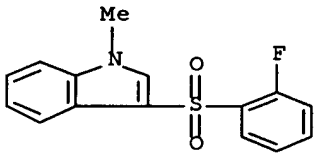
CN 3-Azabicyclo[3.1.0]hexane-6-methanamine, 3-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



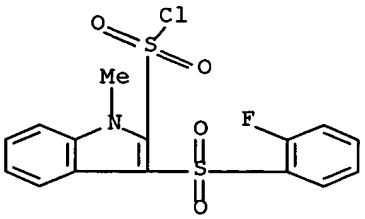
RN 872983-83-0 HCAPLUS
CN Carbamic acid, [[3-[[1-[(2-fluorophenyl)sulfonyl]-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



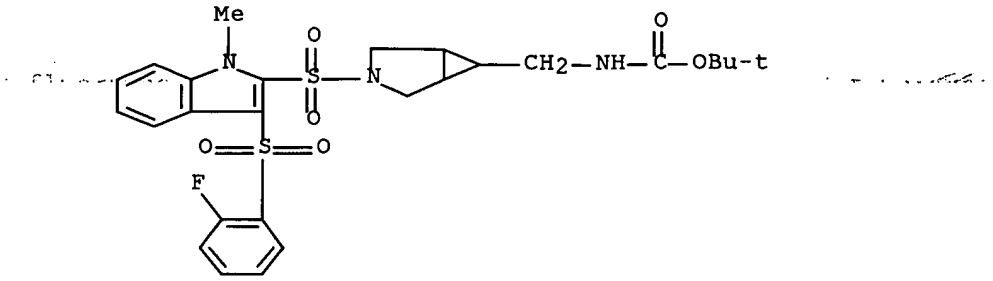
RN 872983-88-5 HCAPLUS
CN 1H-Indole, 3-[(2-fluorophenyl)sulfonyl]-1-methyl- (9CI) (CA INDEX NAME)



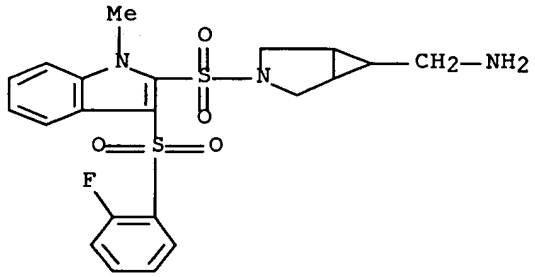
RN 872983-90-9 HCAPLUS
CN 1H-Indole-2-sulfonyl chloride, 3-[(2-fluorophenyl)sulfonyl]-1-methyl- (9CI) (CA INDEX NAME)



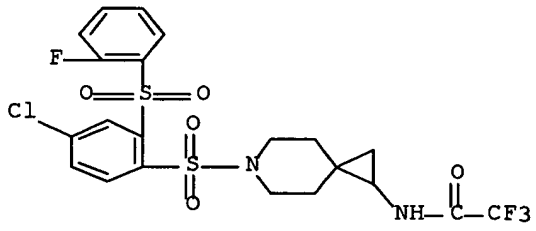
RN 872983-92-1 HCAPLUS
CN Carbamic acid, [[3-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]-3-azabicyclo[3.1.0]hex-6-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



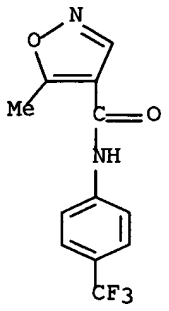
RN 872983-94-3 HCAPLUS
CN 3-Azabicyclo[3.1.0]hexane-6-methanamine, 3-[[3-[(2-fluorophenyl)sulfonyl]-1-methyl-1H-indol-2-yl]sulfonyl]- (9CI) (CA INDEX NAME)



IT 872983-26-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of piperidine derivs. as cannabinoid receptor ligands)
RN 872983-26-1 HCAPLUS
CN Acetamide, N-[6-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-6-azaspiro[2.5]oct-1-yl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

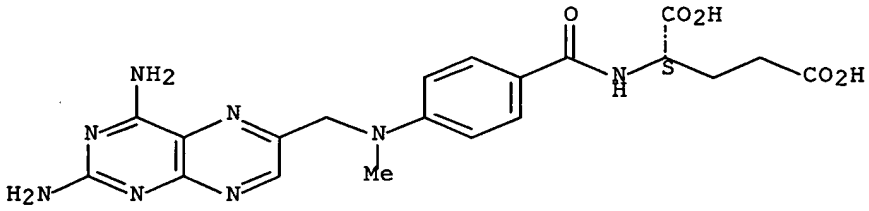


IT 75706-12-6, Leflunomide
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of piperidine derivs. as cannabinoid receptor ligands co-administered with leflunomide)
RN 75706-12-6 HCAPLUS
CN 4-Isoxazolecarboxamide, 5-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



IT 59-05-2, Methotrexate
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of piperidine derivs. as cannabinoid receptor ligands co-administered with methotrexate)
RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

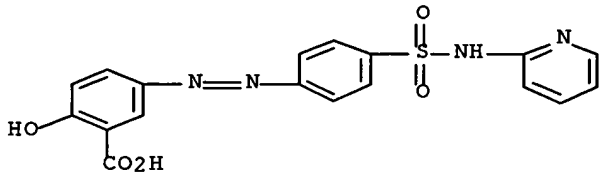
L21 ANSWER 5 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1114244 HCAPLUS Full-text
DOCUMENT NUMBER: 144:285543
TITLE: NanoStore: a concept for logistical improvements of compound handling in high-throughput screening
AUTHOR(S): Benson, Neil; Boyd, Helen F.; Everett, Jeremy R.; Fries, Joachim; Gribbon, Philip; Haque, Nuzrul; Henco, Karsten; Jessen, Timm; Martin, William H.; Mathewson, Travis J.; Sharp, R. Eryl; Spencer, Robin W.; Stuhmeier, Frank; Wallace, Mark S.; Winkler, Dirk
CORPORATE SOURCE: Discovery Biology, Pfizer Global Research and Development, Sandwich, CT13 9NJ, UK
SOURCE: Journal of Biomolecular Screening (2005), 10(6), 573-580
CODEN: JBISF3; ISSN: 1087-0571
PUBLISHER: Sage Publications
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Small mol. screening, the systematic encounter of biol. space with chemical space, has provoked the emergence of a whole industry chat recreates itself by constant iterative improvements to this process. The authors describe an

approach to tackle the problem for one of the most time-consuming steps in the execution of a screening campaign, namely, the reformatting of high-throughput screening test compds. from master plates to daughter assay plates used in the execution of the screen. Through an engineered storage procedure, they prepare plates ahead of the screening process with the resp. compds. in a ready-to-use format. They show the biol. inertness of the method and how it facilitates efficient recovery of compound activity. This uncoupling of normally interconnected processes provides time and compound savings, avoids repeated freeze-thaw cycles of compound solns., and removes the problems associated with the DMSO sensitivity of certain assays types.

IT 599-79-1, Sulfasalazin
RL: ANT (Analyte); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(diverse active compound including sulfasalazin in enzyme, receptor-ligand binding assay could be detected post dry down using nanostore approach where nanostore raised operational efficiency achieved by decoupling compound handling from HTS)

RN 599-79-1 HCAPLUS

CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 6 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1078092 HCAPLUS Full-text

DOCUMENT NUMBER: 143:361162

TITLE: Bacterial small-molecule three-hybrid system based on the interaction of heterodimeric ligand-receptor interaction and use thereof for high-throughput drug screening

INVENTOR(S): Althoff, Eric A.; Cornish, Virginia W.

PATENT ASSIGNEE(S): Trustees of Columbia University In the City of New York, USA

SOURCE: U.S. Pat. Appl. Publ., 28 pp., Cont.-in-part of U.S. Ser. No. 132,039.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005221402	A1	20051006	US 2005-512497	20050523
US 2003203471	A1	20031030	US 2002-132039	20020424
US 7083918	B2	20060801		
WO 2004042345	A2	20040521	WO 2003-US12612	20030424
WO 2004042345	A3	20040923		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-132039 A2 20020424
WO 2003-US12612 W 20030424

OTHER SOURCE(S): MARPAT 143:361162

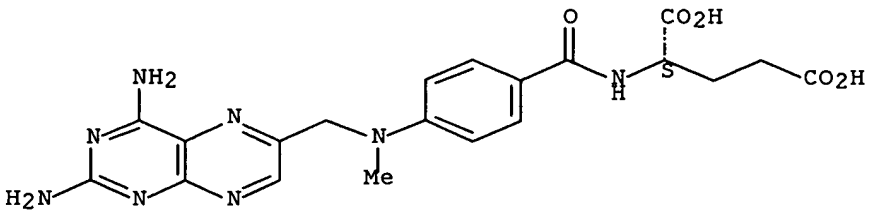
AB A transgenic bacterial cell comprising (a) a dimeric small mol. which comprises a first moiety known to bind a first receptor domain covalently linked to a second moiety known to bind a second receptor domain; (b) nucleotide sequences which upon transcription encode (i) a first fusion protein comprising the first receptor domain, and (ii) a second fusion protein comprising the second receptor domain; and (c) a reporter gene wherein expression of the reporter gene is conditioned on the proximity of the first fusion protein to the second fusion protein. The cell is also adapted for use in a method for identifying a mol. that binds to a known target in a bacterial cell from a pool of candidate mols., and a method for identifying an unknown target receptor to which a mol. is capable of binding in a bacterial cell. Also described are compds. and kits for carrying out the methods, in particular, the synthesis of the Mtx-SLF heterodimer. In particular embodiments, the method is exemplified by using a small mol. heterodimeric Mtx-SLF (methotrexate-SLF(a synthetic analog of FK506)) to bridge the λcI DNA-binding domain, which is fused to FK506 receptor FKBP12 (FK506-binding protein 12), and the activation domain - αNTD (the N-terminal domain of the α-subunit of RNA polymerase), which is fused to methotrexate receptor DHFR (dihydrofolate reductase). The interaction of λcI-FKBP12 and αNTD-DHFR fusion protein leads to the transcription activation of a lacZ reporter gene, in which the λcI binding site is placed upstream of lacZ promoter. Thus, upon addition of the small mol. heterodimer Mtx-SLF, the λcI-FKBP12 and αNTD-DHFR fusion protein are dimerized, which then drives the lacZ transcription. This bacterial small mol. three-hybrid system is useful for high-throughput screening for small mol. drugs and drug-interacting protein targets.

IT 59-05-2P, Methotrexate
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(bacterial small-mol. three-hybrid system based on interaction of heterodimeric ligand-receptor interaction and use thereof for high-throughput drug screening)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 7 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1049799 HCAPLUS Full-text
DOCUMENT NUMBER: 143:319188
TITLE: Treatment of fibrosis using farnesoid X receptor (FXR) ligands
INVENTOR(S): Fiorucci, Stefano; Pellicciari, Roberto; Pruzanski, Mark
PATENT ASSIGNEE(S): Intercept Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005089316	A2	20050929	WO 2005-US8575	20050314
WO 2005089316	A3	20060406		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2006069070	A1	20060330	US 2005-81002	20050314

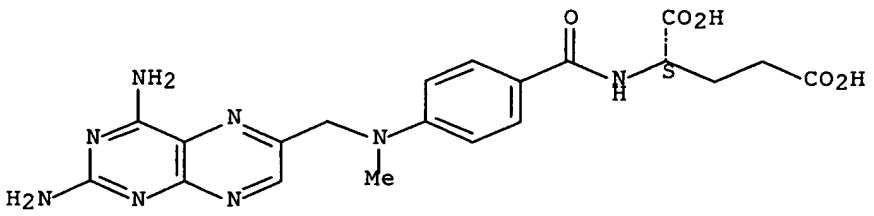
PRIORITY APPLN. INFO.: US 2004-552865P P 20040312

AB The invention discloses a method for inhibiting fibrosis that occurs in an organ where the farnesoid X receptor (FXR) is expressed. The method involves administering a high potency, activating ligand of FXR in an effective amount to a patient who is not suffering from a cholestatic condition. The invention also provides pharmaceutical compns. containing an effective amount of an FXR ligand and kits for dispensing the pharmaceutical compns.

IT 59-05-2, Methotrexate
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (liver disease induced by, liver fibrosis associated with; farnesoid X receptor ligands for treatment of fibrosis)

RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



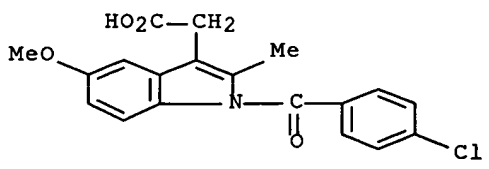
L21 ANSWER 8 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:988973 HCAPLUS Full-text
DOCUMENT NUMBER: 143:339768
TITLE: Identification of Determinants of Ligand Binding Affinity and Selectivity in the Prostaglandin D2 Receptor CRTH2
AUTHOR(S): Hata, Aaron N.; Lybrand, Terry P.; Breyer, Richard M.
CORPORATE SOURCE: Department of Pharmacology, the Vanderbilt Ingram Cancer Center, and the Vanderbilt Center for Structural Biology, Vanderbilt University School of Medicine, Nashville, TN, 37232, USA
SOURCE: Journal of Biological Chemistry (2005), 280(37), 32442-32451
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The chemoattractant receptor-homologous mol. expressed on Th2 cells (CRTH2) is a G protein-coupled receptor that mediates the pro-inflammatory effects of prostaglandin D2 (PGD2) generated in allergic inflammation. The CRTH2 receptor shares greatest sequence similarity with chemoattractant receptors compared with prostanoid receptors. To investigate the structural determinants of CRTH2 ligand binding, the authors performed site-directed mutagenesis of putative mCRTH2 ligand-binding residues, and the authors evaluated mutant receptor ligand binding and functional properties. Substitution of alanine at each of three residues in the transmembrane (TM) helical domains (His 106, TM III; Lys 209, TM V; and Glu 268, TM VI) and one in extracellular loop II (Arg 178) decreased PGD2 binding affinity, suggesting that these residues play a role in binding PGD2. In contrast, the H106A and E268A mutants bound indomethacin, a nonsteroidal anti-inflammatory drug, with an affinity similar to the wild-type receptor. HEK293 cells expressing the H106A, K209A, and E268A mutants displayed reduced inhibition of intracellular cAMP and chemotaxis in response to PGD2, whereas the H106A and E268A mutants had functional responses to indomethacin similar to the wild-type receptor. Binding of PGE2 by the E268A mutant was enhanced compared with the wild-type receptor, suggesting that Glu 268 plays a role in determining prostanoid ligand selectivity. Replacement of Tyr 261 with phenylalanine did not affect PGD2 binding but decreased the binding affinity for indomethacin. These results provided the first details of the ligand binding pocket of an eicosanoid-binding chemoattractant receptor.

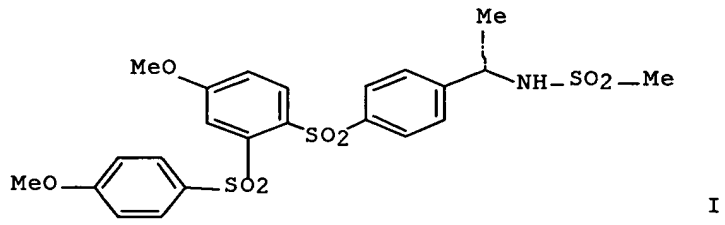
IT 53-86-1, Indomethacin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(identification of determinants of ligand binding affinity and selectivity in murine prostaglandin D2 receptor CRTH2)

RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 9 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:980797 HCAPLUS Full-text
DOCUMENT NUMBER: 143:318371
TITLE: Triaryl bis-sulfones as cannabinoid-2 receptor ligands: SAR studies
AUTHOR(S): Shankar, Bandarpalle B.; Lavey, Brian J.; Zhou, Guowei; Spitler, James A.; Tong, Ling; Rizvi, Razia; Yang, De-Yi; Wolin, Ronald; Kozlowski, Joseph A.; Shih, Neng-Yang; Wu, Jie; Hipkin, R. William; Gonsiorek, Waldemar; Lunn, Charles A.
CORPORATE SOURCE: Department of Chemistry, Schering-Plough Research Institute, Kenilworth, NJ, 07033-0539, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(20), 4417-4420
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



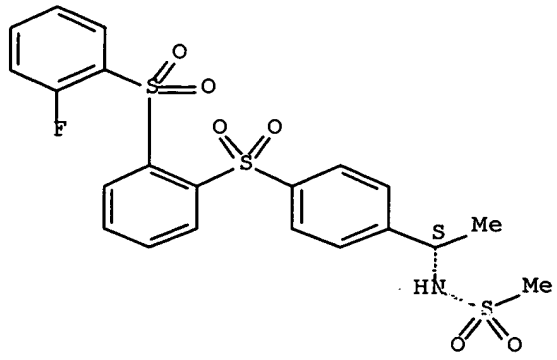
I

AB The authors recently reported that compound (I) is a potent inhibitor of the CB2 receptor with high selectivity over CB1. This paper describes the SAR development for this class of compds. Variation of the substitution pattern on the aromatic rings, as well as the groups linking them together, led to sub-nanomolar inhibitors of the CB2 receptor, with high selectivity over CB1.

IT 447459-45-2P 447459-54-3P 447459-65-6P
447459-74-7P 864872-45-7P 864872-46-8DP,
derivs. 864872-47-9P 864872-48-0P 864872-49-1P
864872-50-4P 864872-51-5P 864872-52-6P
864872-53-7P 864872-54-8P 864872-55-9P
864872-56-0P 864872-57-1P 864872-58-2P
864872-59-3P 864872-60-6P 864872-61-7P
864872-62-8P 864872-63-9P 864872-64-0P
864872-65-1P 864872-66-2P 864872-67-3P
864872-68-4P 864872-69-5P 864872-70-8P
864872-71-9P 864872-72-0P 864872-73-1P
864872-74-2P 864872-75-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(SAR studies of triaryl bis-sulfones as cannabinoid-2 receptor ligands)

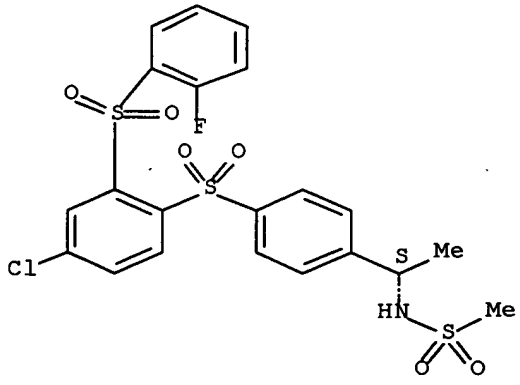
RN 447459-45-2 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



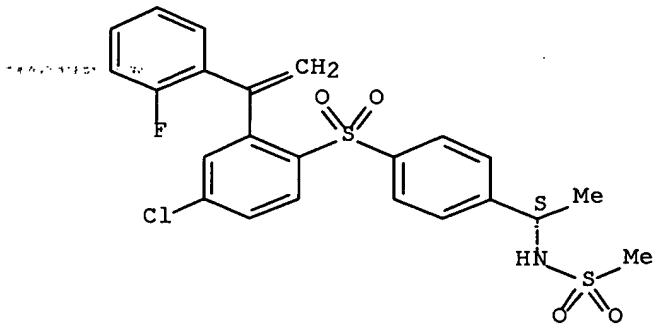
RN 447459-54-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



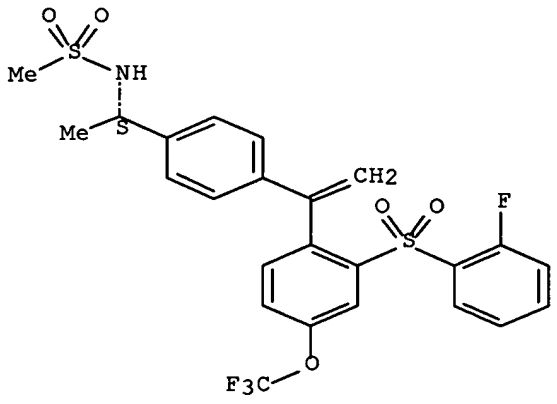
RN 447459-65-6 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[1-(2-fluorophenyl)ethenyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



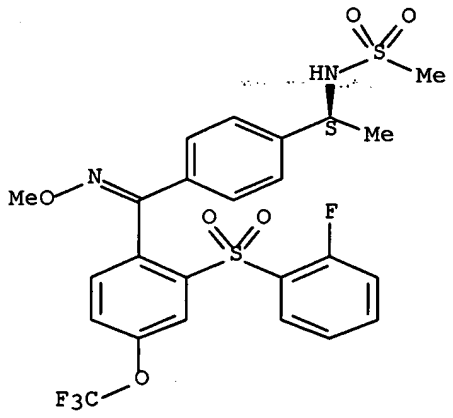
RN 447459-74-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[1-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]ethenyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



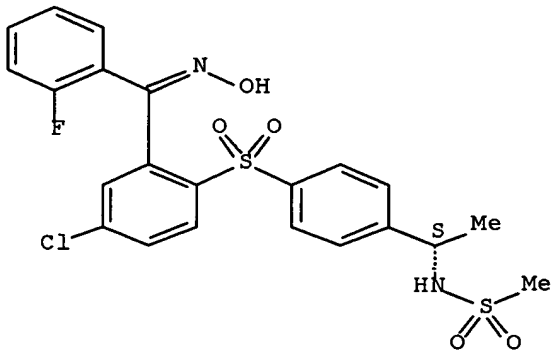
RN 864872-45-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl](methoxyimino)methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



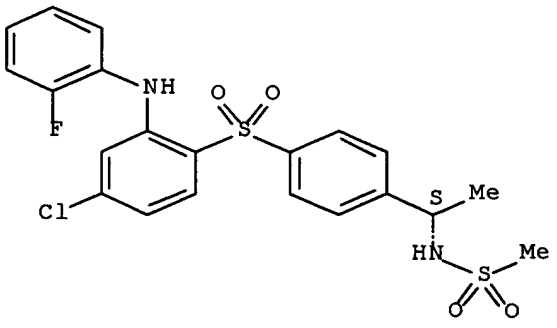
RN 864872-46-[illegible] HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)(hydroxyimino)methyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



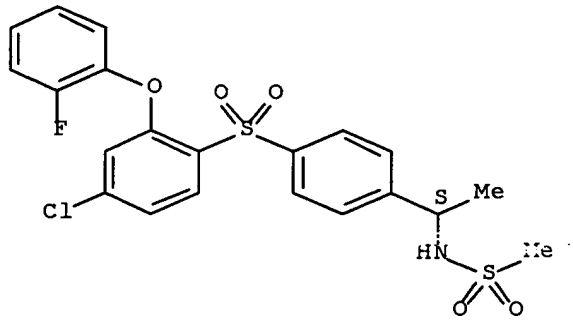
RN 864872-47-9 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)amino]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



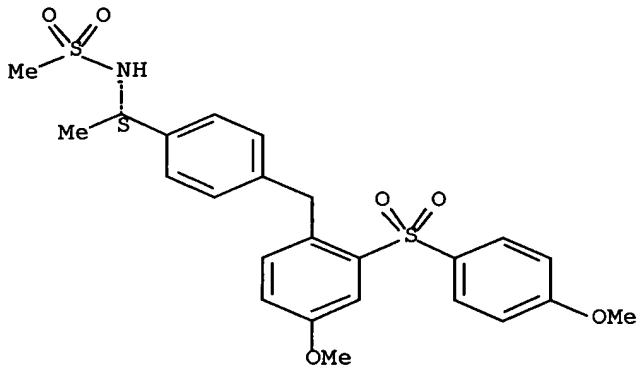
RN 864872-48-0 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(2-fluorophenoxy)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



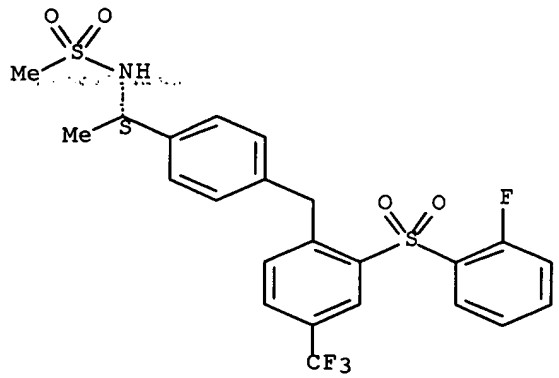
RN 864872-49-1 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



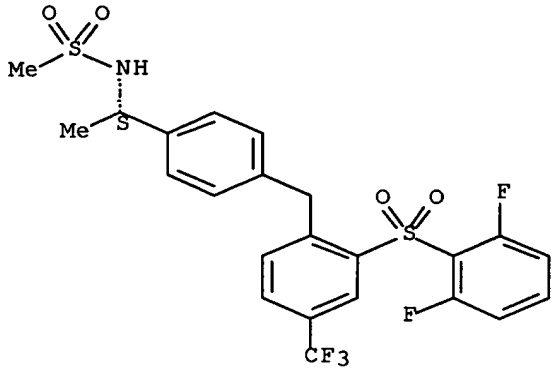
RN 864872-50-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



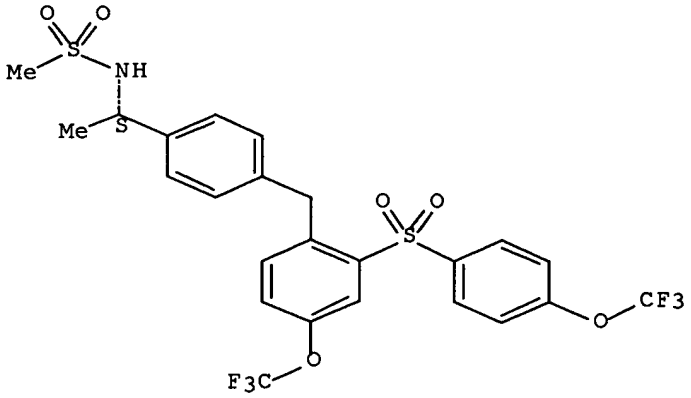
RN 864872-51-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2,6-difluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



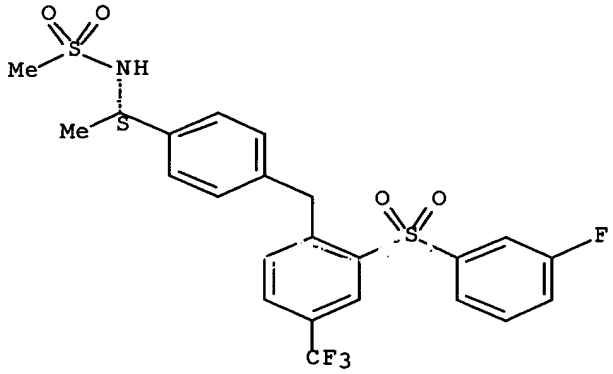
RN 864872-52-6 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-(trifluoromethoxy)-2-[[4-(trifluoromethoxy)phenyl]sulfonyl]phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



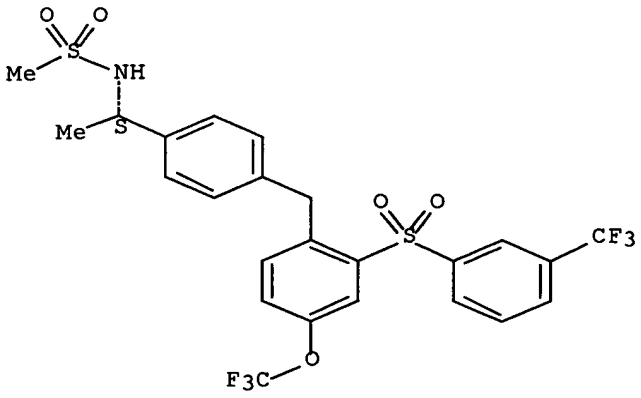
RN 864872-53-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(3-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



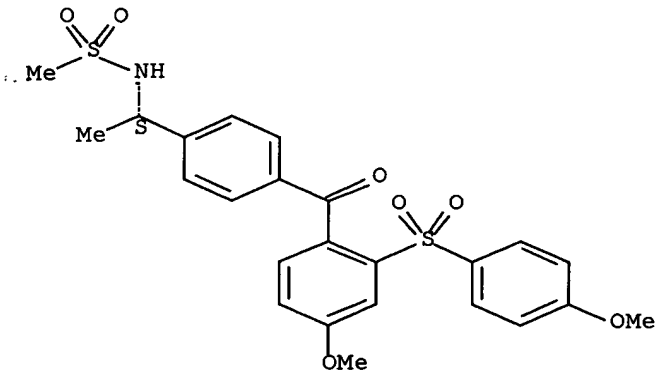
RN 864872-54-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-(trifluoromethoxy)-2-[[3-(trifluoromethyl)phenyl]sulfonyl]phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



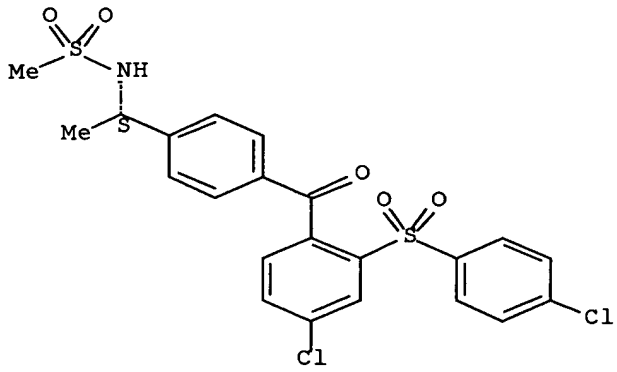
RN 864872-55-9 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



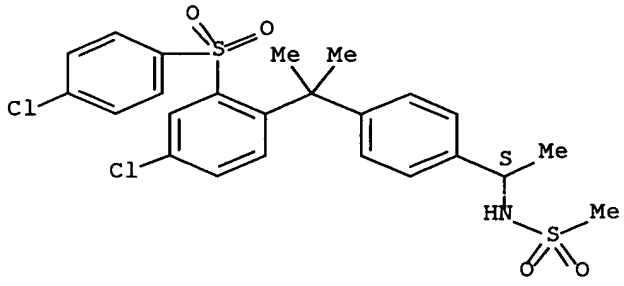
RN 864872-56-0 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[4-chloro-2-[(4-chlorophenyl)sulfonyl]benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 864872-57-1 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[1-[4-chloro-2-[(4-chlorophenyl)sulfonyl]phenyl]-1-methylethyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

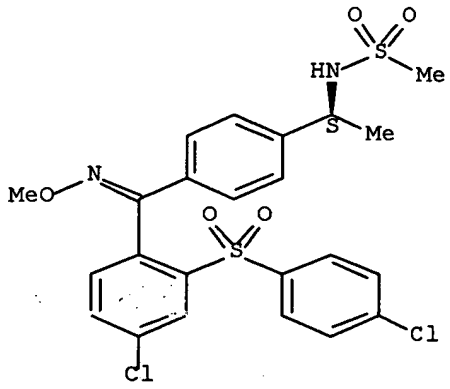
Absolute stereochemistry.



RN 864872-58-2 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(4-

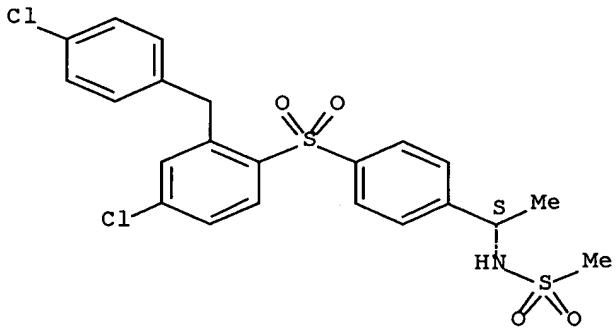
chlorophenyl)sulfonyl]phenyl](methoxyimino)methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



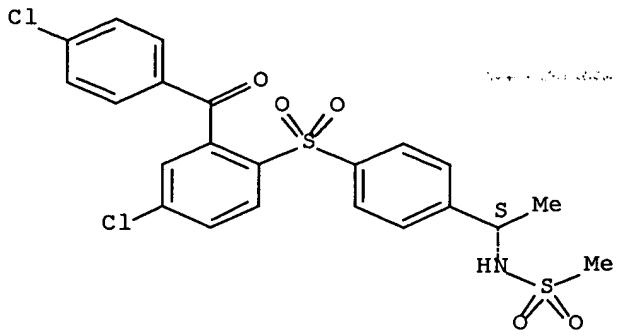
RN 864872-59-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(4-chlorophenyl)methyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



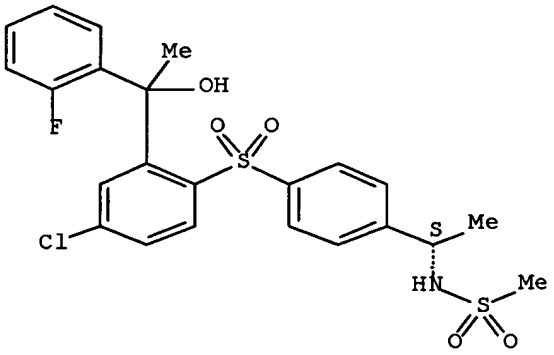
RN 864872-60-6 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(4-chlorobenzoyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



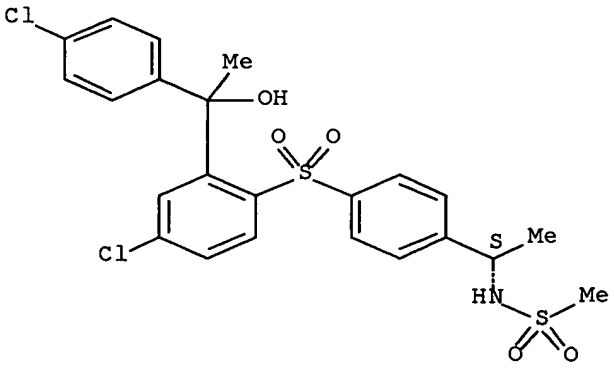
RN 864872-61-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[1-(2-fluorophenyl)-1-hydroxyethyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 864872-62-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[1-(4-chlorophenyl)-1-hydroxyethyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

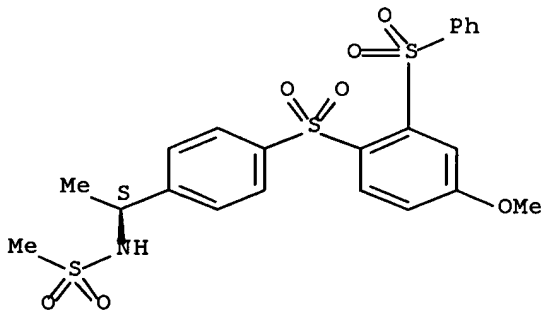
Absolute stereochemistry.



RN 864872-63-9 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[4-methoxy-2-(phenylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

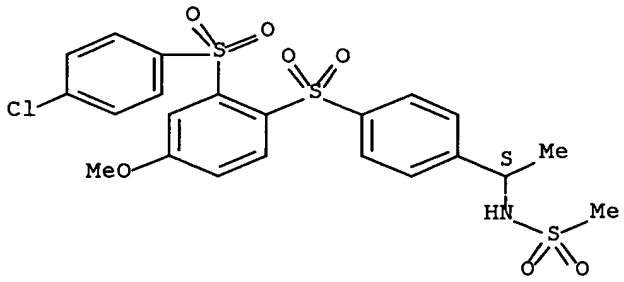
Absolute stereochemistry.



RN 864872-64-0 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

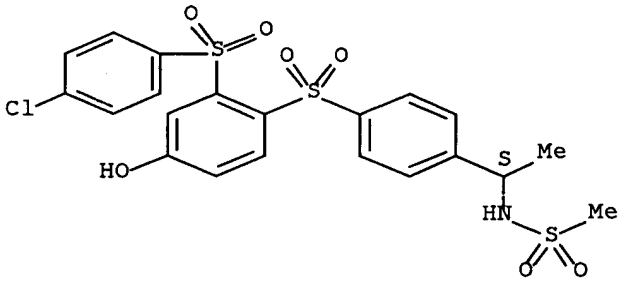
Absolute stereochemistry.



RN 864872-65-1 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-hydroxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

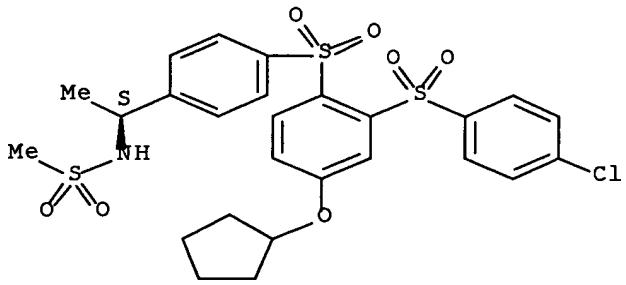
Absolute stereochemistry.



RN 864872-66-2 HCAPLUS

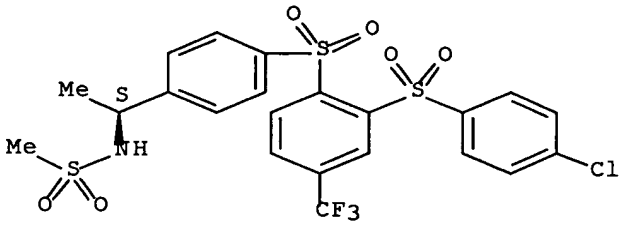
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-(cyclopentyloxy)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



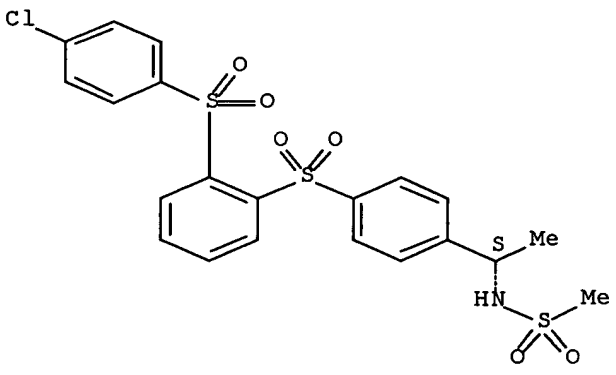
RN 864872-67-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



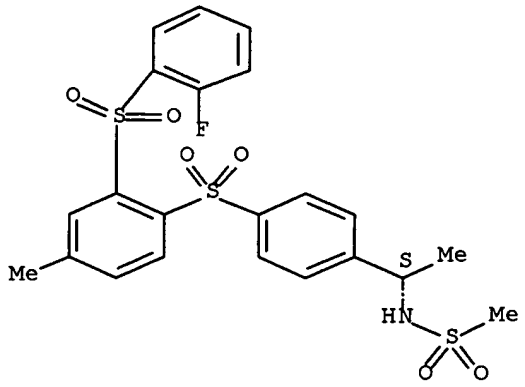
RN 864872-68-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



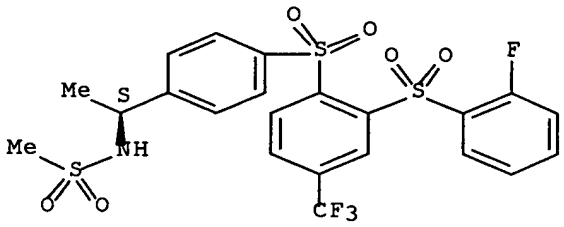
RN 864872-69-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-methylphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



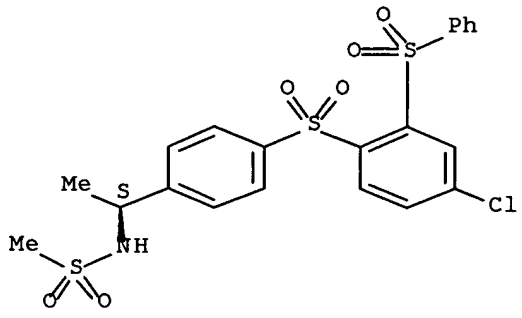
RN 864872-70-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 864872-71-9 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(phenylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

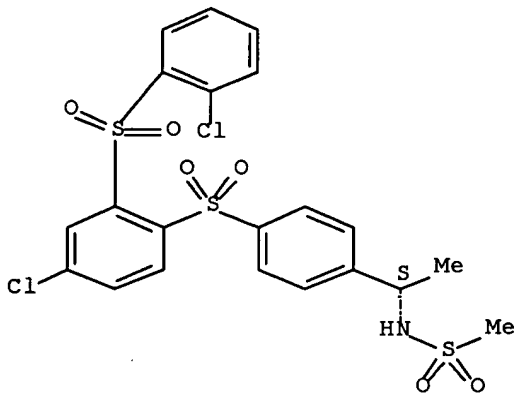
Absolute stereochemistry.



RN 864872-72-0 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-chlorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX

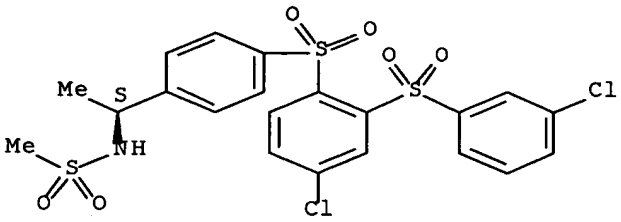
NAME)

Absolute stereochemistry.



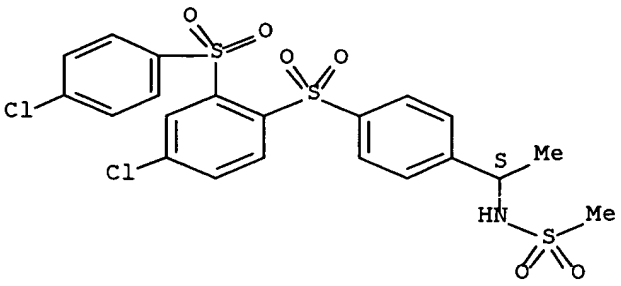
RN 864872-73-1 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(3-chlorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 864872-74-2 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(4-chlorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

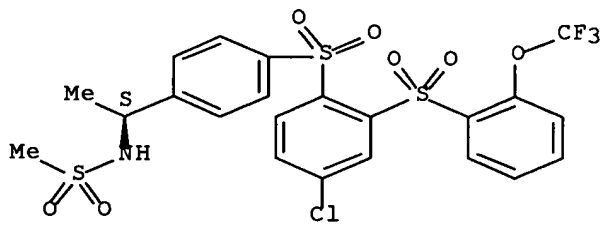
Absolute stereochemistry.



RN 864872-75-3 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[[2-(trifluoromethoxy)phenyl]sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

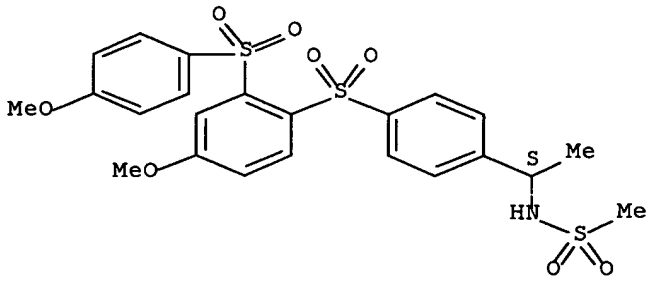


IT 447459-51-0 864872-90-2 864872-91-3
864872-92-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(SAR studies of triaryl bis-sulfones as cannabinoid-2 receptor ligands)

RN 447459-51-0 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

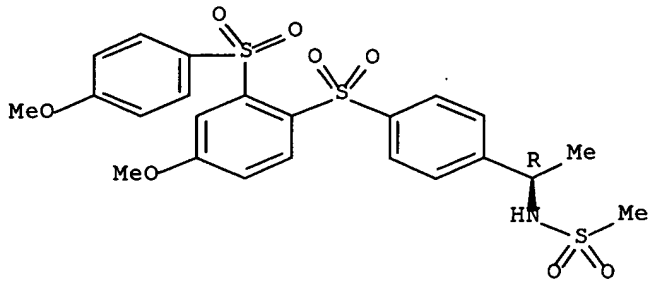
Absolute stereochemistry.



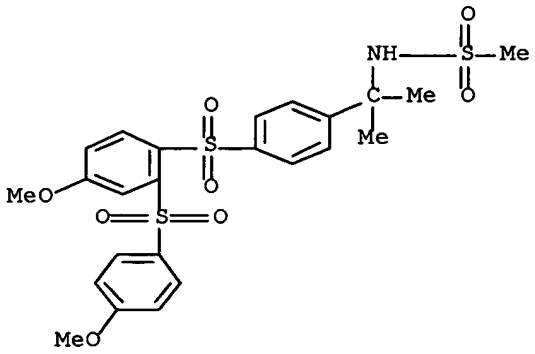
RN 864872-90-2 HCAPLUS

CN Methanesulfonamide, N-[(1R)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

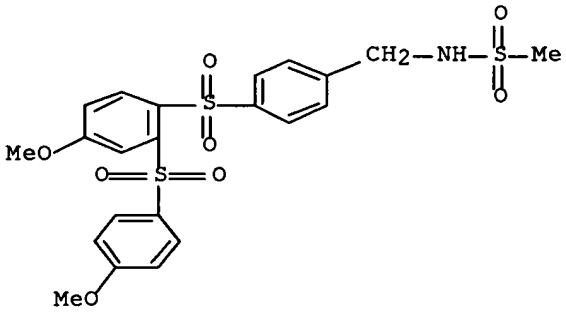
Absolute stereochemistry.



RN 864872-91-3 HCAPLUS
CN Methanesulfonamide, N-[1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]-1-methylethyl]- (9CI) (CA INDEX NAME)



RN 864872-92-4 HCAPLUS
CN Methanesulfonamide, N-[[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

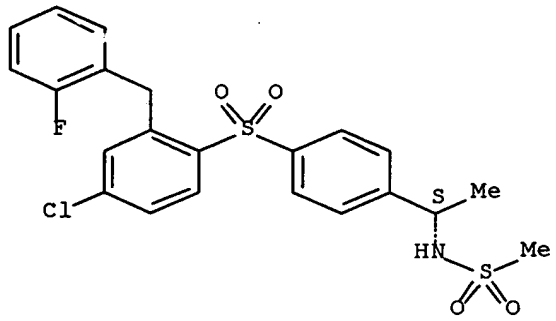


IT 447459-63-4P 447459-64-5P 447459-97-4P
447460-00-6P 447460-01-7P 447460-03-9P
447460-11-9P 447460-12-0P 447460-17-5P
447460-19-7P 447460-24-4P 447460-28-8P
447460-49-3P 447460-51-7P 864872-44-6P
864872-79-7P 864872-80-0P 864872-81-1P

864872-82-2P 864872-83-3P 864872-84-4P
864872-85-5P 864872-86-6P 864872-87-7P
864872-88-8P 864872-89-9P 864872-93-5P
864872-94-6P 864872-95-7P 864872-96-8P
864872-97-9P 864872-98-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(SAR studies of triaryl bis-sulfones as cannabinoid-2 receptor ligands)

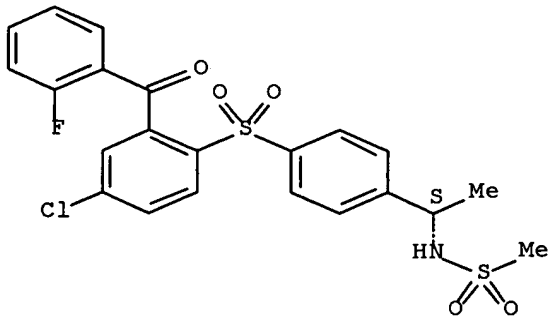
RN 447459-63-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)methyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



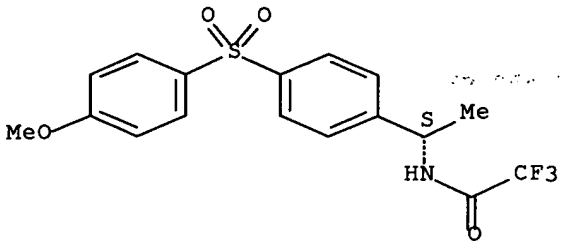
RN 447459-64-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(2-fluorobenzoyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



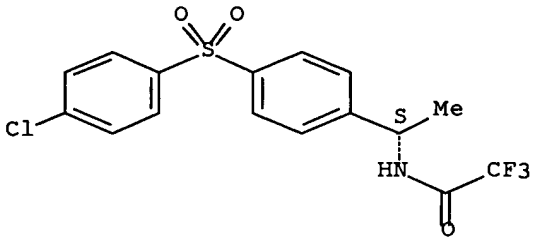
RN 447459-97-4 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[(4-methoxyphenyl)sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



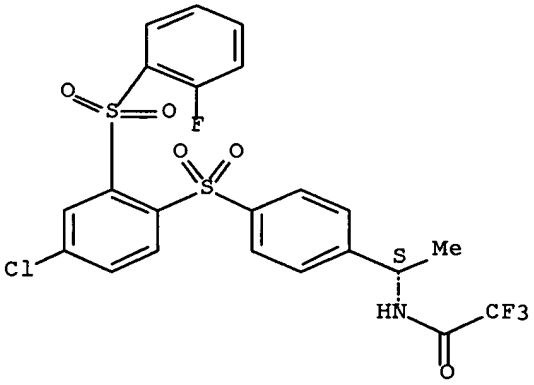
RN 447460-00-6 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chlorophenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



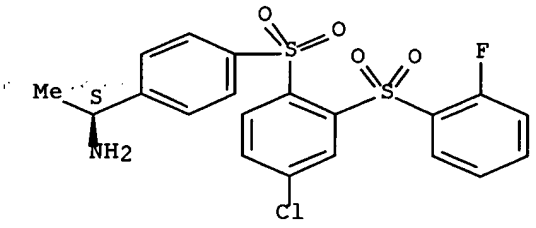
RN 447460-01-7 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



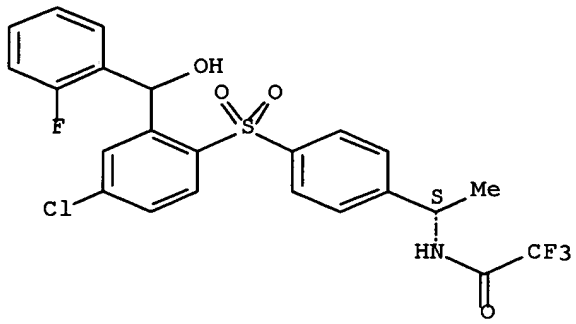
RN 447460-03-9 HCAPLUS
CN Benzenemethanamine, 4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



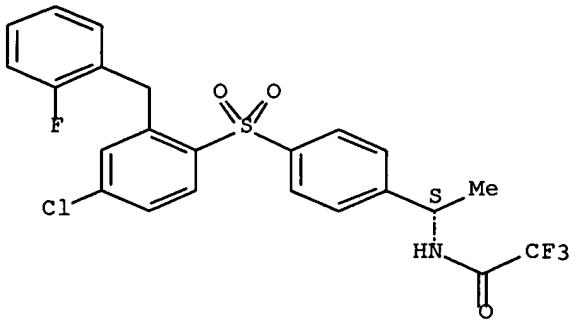
RN 447460-11-9 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)hydroxymethyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



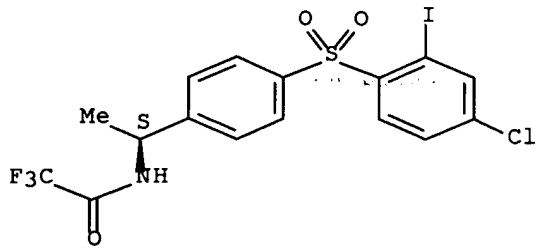
RN 447460-12-0 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)methyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

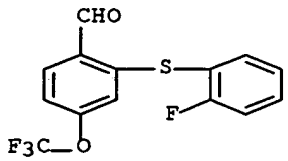


RN 447460-17-5 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chloro-2-iodophenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

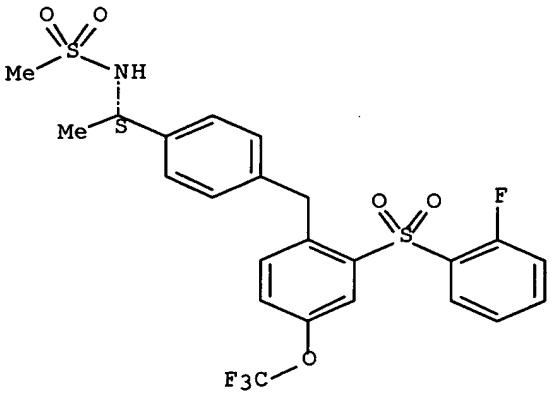


RN 447460-19-7 HCAPLUS
CN Benzaldehyde, 2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



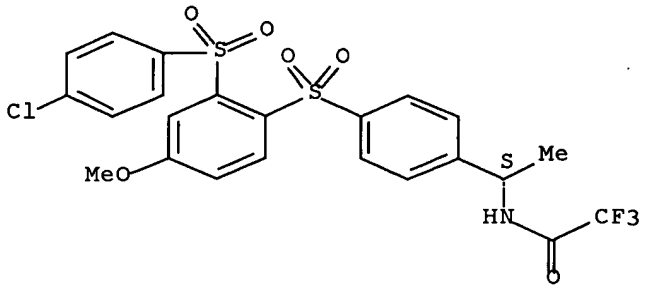
RN 447460-24-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



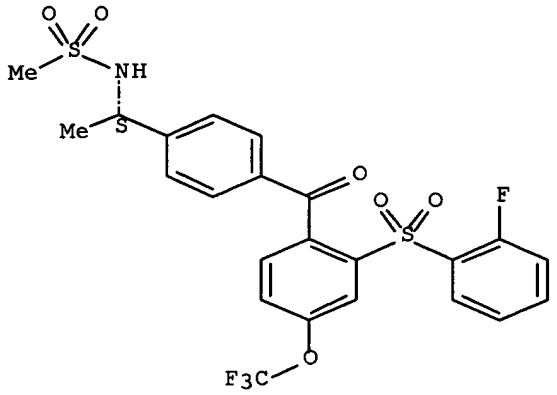
RN 447460-28-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



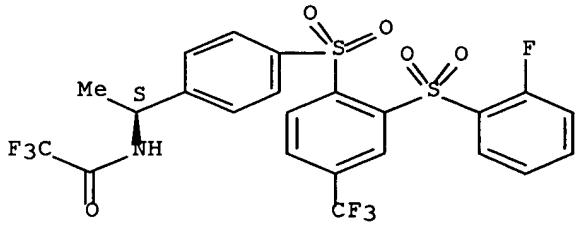
RN 447460-49-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



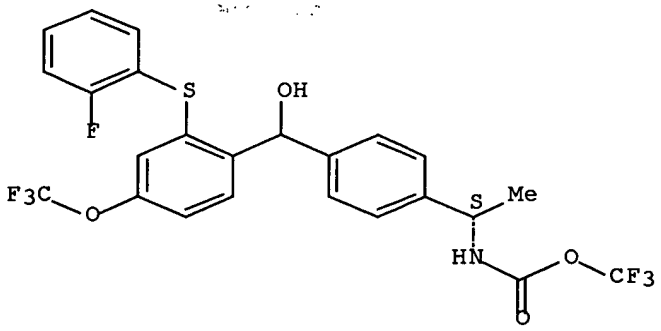
RN 447460-51-7 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



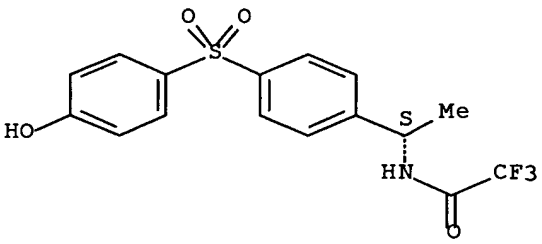
RN 864872-44-6 HCAPLUS
CN Carbamic acid, [(1S)-1-[4-[[2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)phenyl]hydroxymethyl]phenyl]ethyl]-, trifluoromethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



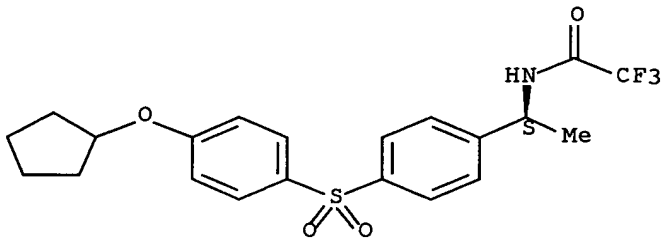
RN 864872-79-7 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[(4-hydroxyphenyl)sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



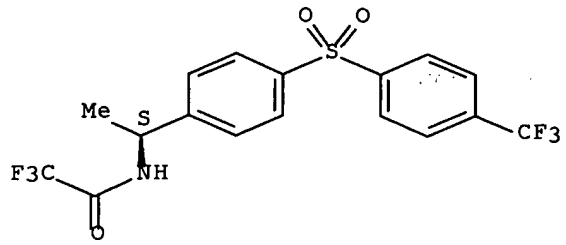
RN 864872-80-0 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-(cyclopentyloxy)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



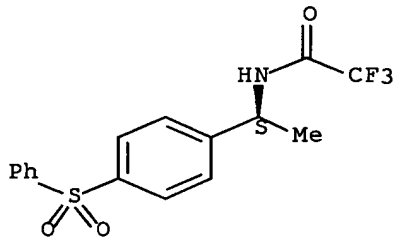
RN 864872-81-1 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



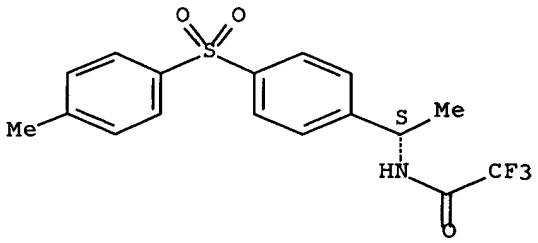
RN 864872-82-2 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-(phenylsulfonyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



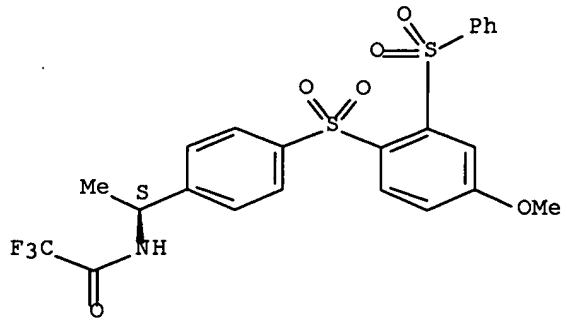
RN 864872-83-3 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[(4-methylphenyl)sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



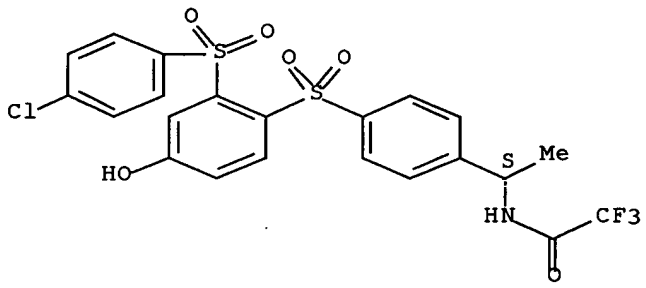
RN 864872-84-4 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[4-methoxy-2-(phenylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



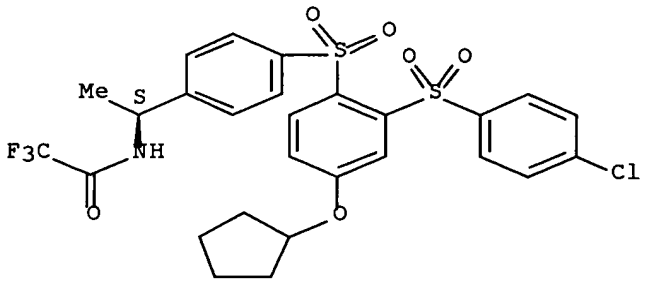
RN 864872-85-5 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-hydroxyphenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



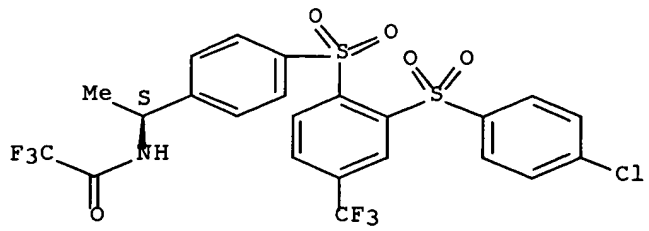
RN 864872-86-6 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-(cyclopentyloxy)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



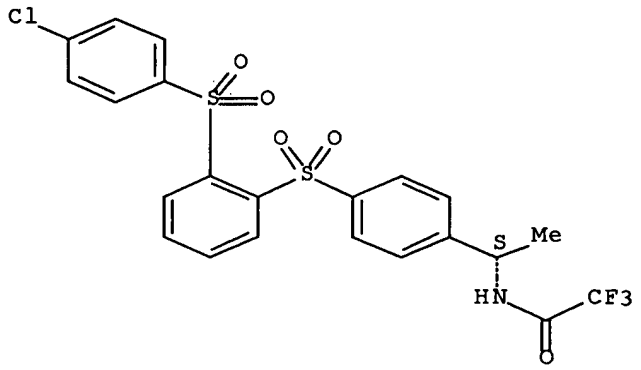
RN 864872-87-7 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



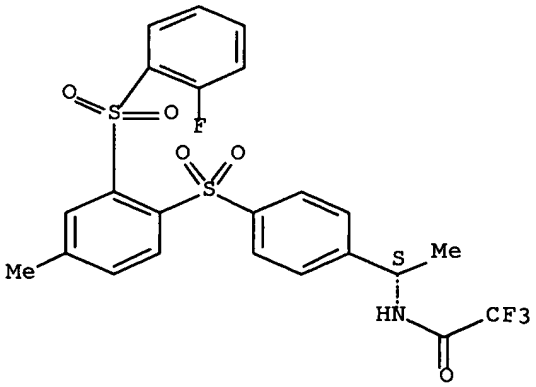
RN 864872-88-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]phenyl]sulfonyl]phenylethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



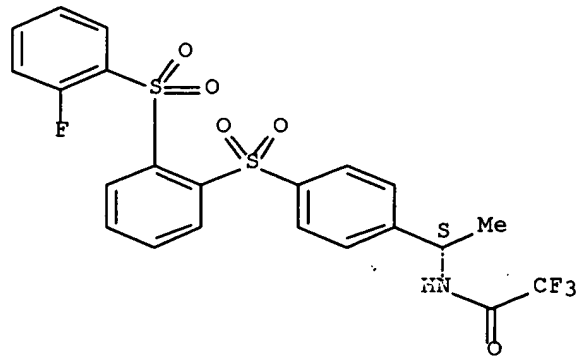
RN 864872-89-9 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-methylphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



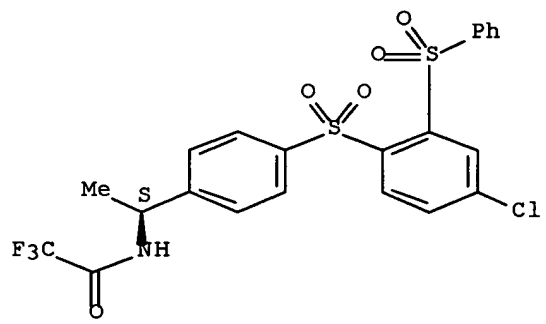
RN 864872-93-5 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



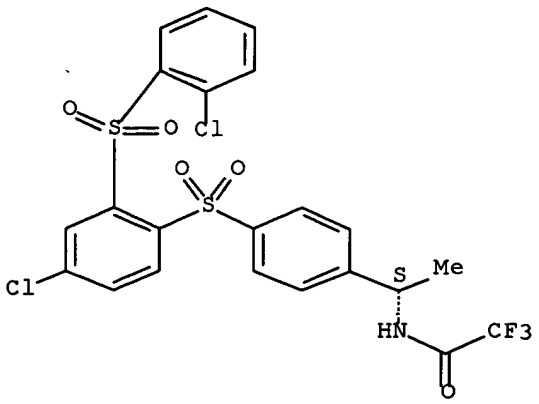
RN 864872-94-6 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-(phenylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



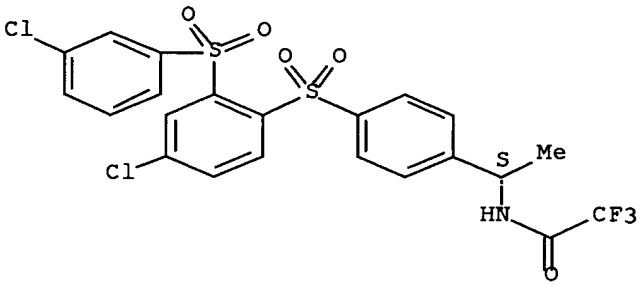
RN 864872-95-7 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-chlorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



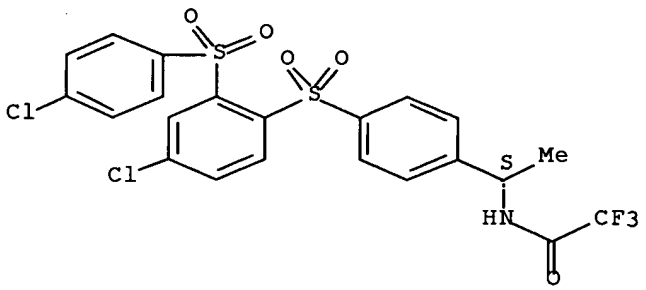
RN 864872-96-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(3-chlorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



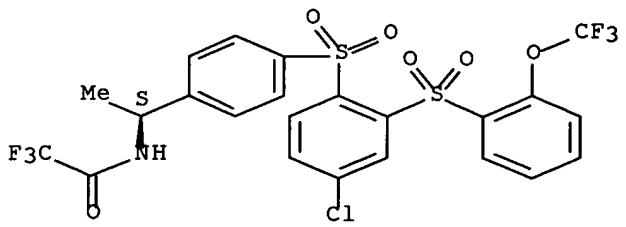
RN 864872-97-9 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(4-chlorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 864872-98-0 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[[2-(trifluoromethoxy)phenyl]sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 10 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:823681 HCAPLUS Full-text
DOCUMENT NUMBER: 143:216704
TITLE: Crystalline polymorphs of a CXC-chemokine receptor ligand
INVENTOR(S): Hu, Mengwei; Yu, Younong; Dwyer, Michael; Taveras, Arthur G.; Kim-Meade, Agnes; Yin, Jianguo; Fu, Xiaoyong; Mcallister, Timothy; Zhang, Shuyi; Klopfer, Kevin
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

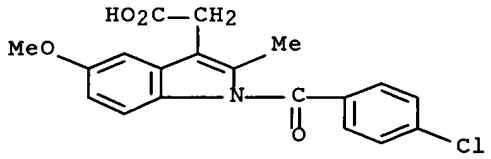
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005075447	A1	20050818	WO 2005-US3414	20050128
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005192345	A1	20050901	US 2005-45772	20050128
PRIORITY APPLN. INFO.:			US 2004-540487P	P 20040130

AB The present invention relates to 4 distinct crystalline polymorphs of a monohydrate of 2-hydroxy-N,N-dimethyl-3-[[2-[[1-(5-methyl-2-furanyl)propyl]amino]-3,4-dioxo-1-cyclobuten-1-yl]amino]benzamide. These 4 polymorphic forms, herein referred to as Forms I, II, III and IV are active as a CXC-chemokine receptor ligands. The invention is further directed to formulations, methods of treatment, and processes of synthesis of these polymorphic forms.

IT 53-86-1, Indomethacin 59-05-2, Methotrexate
599-79-1, Sulfasalazine 75706-12-6, Leflunimide
162011-90-7, Rofecoxib 169590-42-5, Celecoxib

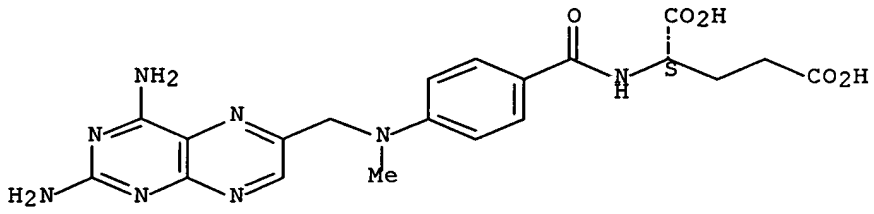
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(crystalline polymorphs of CXC-chemokine receptor ligand
)

RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)

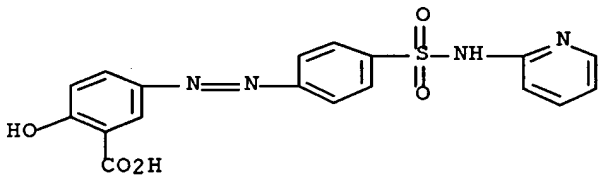


RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

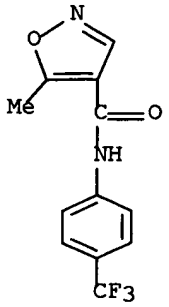
Absolute stereochemistry.



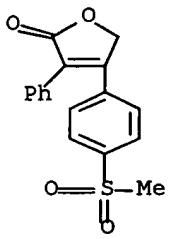
RN 599-79-1 HCAPLUS
CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)



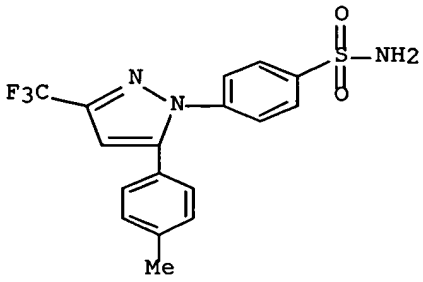
RN 75706-12-6 HCAPLUS
CN 4-Isoxazolecarboxamide, 5-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 162011-90-7 HCAPLUS
CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 169590-42-5 HCAPLUS
CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 11 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:673292 HCAPLUS Full-text
DOCUMENT NUMBER: 143:172866
TITLE: Preparation of isothiazole dioxides as CXC- and CC-chemokine receptor ligands
INVENTOR(S): Taveras, Arthur G.; Zheng, Junying; Biju, Purakkattle J.; Yu, Younong; Chao, Jianhua; Fine, Jay; Lundell, Daniel; Priestley, Tony; Reggiani, Angelo; Merritt, J.

	Robert; Baldwin, John J.; Lai, Gaifa; Wu, Minglang
PATENT ASSIGNEE(S):	Schering Corporation, USA; Pharmacopeia Drug Discovery, Inc.
SOURCE:	PCT Int. Appl., 427 pp.
	CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005068460	A1	20050728	WO 2004-US42720	20041220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2006025453	A1	20060202	US 2004-17505	20041220
PRIORITY APPLN. INFO.:			US 2003-531693P P	20031222
OTHER SOURCE(S):	MARPAT 143:172866			

GI

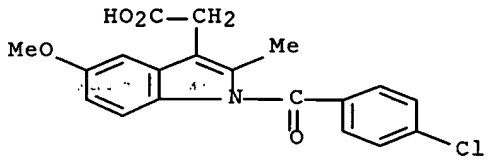
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Disclosed are novel compds. I [D, E = N, CR50; provided that D and E are not the same (one is N and the other is CR50); R50 = H, CF3, CN, etc.; A = (hetero)aryl, (hetero)arylalkyl; B = (hetero)aryl] and the pharmaceutically acceptable salts and solvates thereof. Also disclosed is a method of treating a chemokine mediated diseases, such as, cancer, angiogenesis, angiogenic ocular diseases, pulmonary diseases, multiple sclerosis, rheumatoid arthritis, osteoarthritis, stroke and cardiac reperfusion injury, pain (e.g., acute pain, acute and chronic inflammatory pain, and neuropathic pain) using a compound I. Although the methods of preparation are not claimed, hundreds of example prepns. and/or characterization data are included. For example, II was prepared in 68% yield from the isothiazoledioxide III and the amine IV.pTSA (preparation of reactants given). Antagonist activities of some examples of I towards CXCR1, CXCR2 and CCR7 are given.

IT 53-86-1, Indomethacin 59-05-2, Methotrexate
599-79-1, Sulfasalazine 75706-12-6, Leflunomide
162011-90-7, Rofecoxib 169590-42-5, Celecoxib
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(co-drug; preparation of isothiazole dioxides as CXC- and CC-chemokine receptor ligands)

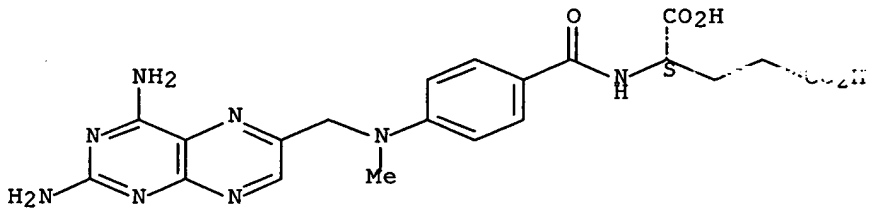
RN 53-86-1 HCAPLUS

CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)

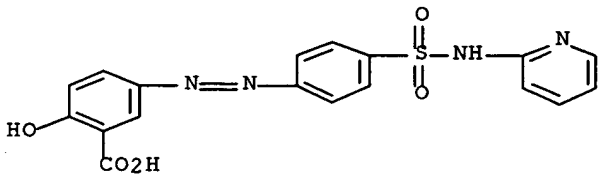


RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

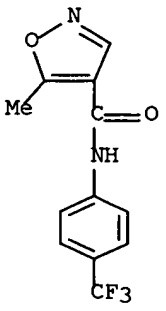
Absolute stereochemistry.



RN 599-79-1 HCAPLUS
CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)

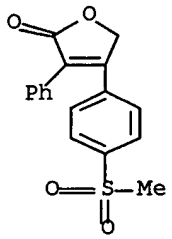


RN 75706-12-6 HCAPLUS
CN 4-Isoxazolecarboxamide, 5-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



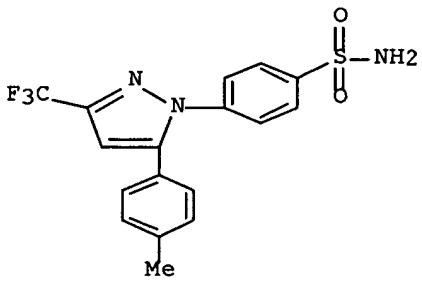
RN 162011-90-7 HCAPLUS

CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 169590-42-5 HCAPLUS

CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 12 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:638859 HCAPLUS Full-text

DOCUMENT NUMBER: 143:153384

TITLE: Preparation of diaminothiadiazoles as CXC- and CC-chemokine receptor ligands

INVENTOR(S): Biju, Purakkattle J.; Taveras, Arthur G.; Yu, Younong; Zheng, Junying; Chao, Jianhua; Aki, Cynthia J.; Fine, Jay; Lundell, Daniel; Priestley, Tony; Reggiani, Angelo; Merritt, J. Robert; Baldwin, John J.

PATENT ASSIGNEE(S): Schering Corporation, USA; Pharmacopeia Drug Discovery, Inc.

SOURCE: PCT Int. Appl., 593 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005066147	A1	20050721	WO 2004-US42060	20041216

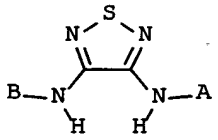
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-531311P P 20031219
US 2003-531713P P 20031222

OTHER SOURCE(S): MARPAT 143:153384

GI



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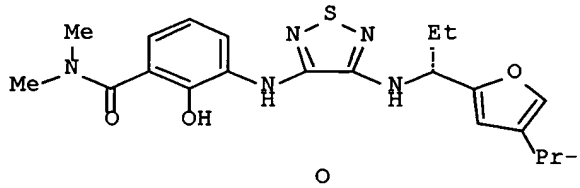

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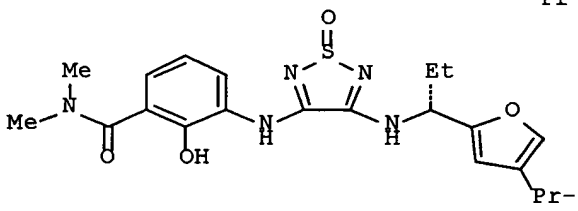


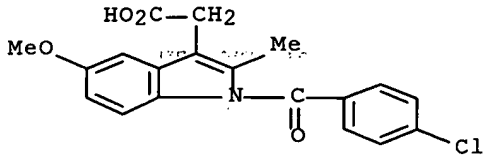
III

AB Disclosed are diaminothiadiazoles I [A = (hetero)aryl, (hetero)arylmethyl (substituted at CH2), etc.; B = (hetero)aryl] and the pharmaceutically acceptable salts and solvates thereof. Also disclosed is a method of treating a chemokine mediated diseases, such as, cancer, angiogenesis, angiogenic ocular diseases, pulmonary diseases, multiple sclerosis, rheumatoid arthritis, osteoarthritis, stroke and ischemia reperfusion injury, acute pain, acute and chronic inflammatory pain, and neuropathic pain using I. Although the methods of preparation are not claimed, hundreds of example prepns. and/or characterization data are included. For example, II was prepared in 43% yield from its monooxide III (preparation given). Antagonist activities of some examples of I towards CXCR1, CXCR2 and CCR7 are given.

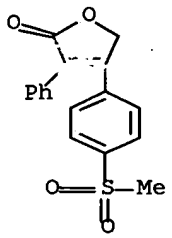
IT 53-86-1, Indomethacin 162011-90-7, Rofecoxib
169590-42-5, Celecoxib
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(co-drug; preparation of diaminothiadiazoles as CXC- and CC-chemokine receptor ligands)

RN 53-86-1 HCAPLUS

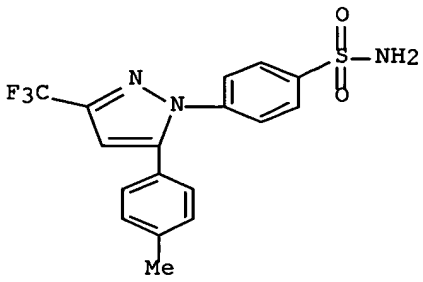
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



RN 162011-90-7 HCAPLUS
CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)

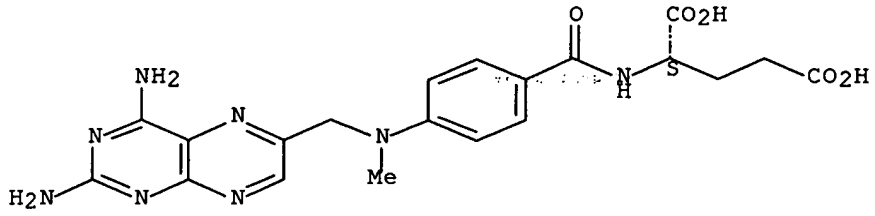


RN 169590-42-5 HCAPLUS
CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

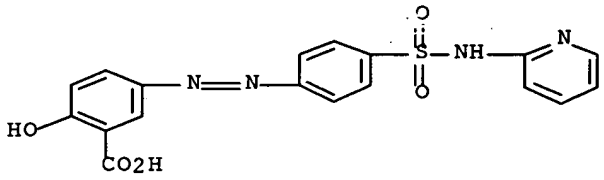


IT 59-05-2 599-79-1 75706-12-6
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(codrug for multiple sclerosis; preparation of diaminothiadiazoles as CXC- and CC-chemokine receptor ligands)
RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

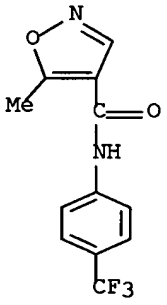
Absolute stereochemistry.



RN 599-79-1 HCAPLUS
CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)



RN 75706-12-6 HCAPLUS
CN 4-Isoxazolecarboxamide, 5-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 13 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:636158 HCAPLUS Full-text
DOCUMENT NUMBER: 143:205794
TITLE: A physicogenetic method to assign ligand-binding relationships between 7TM receptors
AUTHOR(S): Frimurer, Thomas M.; Ulven, Trond; Elling, Christian E.; Gerlach, Lars-Ole; Kostenis, Evi; Hoegberg, Thomas
CORPORATE SOURCE: 7TM Pharma A/S, Horsholm, DK-2970, Den.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(16), 3707-3712
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.

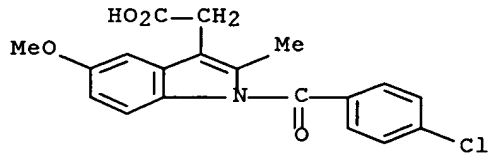
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A computational protocol has been devised to relate 7TM receptor proteins (GPCRs) with respect to physicochem. features of the core ligand-binding site as defined from the crystal structure of bovine rhodopsin. The identification of such receptors that already are associated with ligand information (e.g., small mol. ligands with mutagenesis or SAR data) is used to support structure-guided drug design of novel ligands. A case targeting the newly identified prostaglandin D2 receptor CRTH2 serves as a primary example to illustrate the procedure.

IT 53-86-1, Indometacin
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(physicogenetic method to assign ligand-binding relationships between 7TM receptors)

RN 53-86-1 HCAPLUS

CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 14 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:405367 HCAPLUS Full-text
DOCUMENT NUMBER: 142:441852
TITLE: Compounds and method for treating cancer
INVENTOR(S): McTavish, Hugh
PATENT ASSIGNEE(S): IGF Oncology, LLC, USA
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005041865	A2	20050512	WO 2004-US34704	20041021
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2542834	AA	20050512	CA 2004-2542834	20041021

EP 1680073 A2 20060719 EP 2004-795814 20041021
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRIORITY APPLN. INFO.: US 2003-513048P P 20031021
WO 2004-US34704 W 20041021

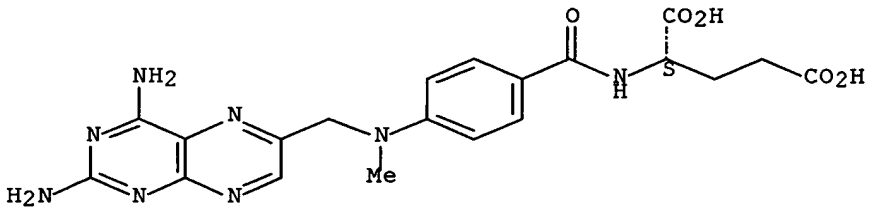
AB The invention provides a method of treating cancer involving administration of an insulin-like growth factor-1 receptor (IGF-1 receptor) agonist and an anticancer chemotherapeutic agent. Also provided are compds. for treating cancer comprising an IGF-1-receptor ligand coupled to an anticancer chemotherapeutic agent. Also provided are compds. for treating cancer comprising an insulin-receptor ligand coupled to an anticancer chemotherapeutic agent.

IT 59-05-2D, Methotrexate, conjugates with insulin receptor ligand
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compds. and method for treating cancer)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 15 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:906860 HCAPLUS Full-text
DOCUMENT NUMBER: 141:374603
TITLE: Human adipocyte fatty acid-binding protein (aP2) gene promoter-driven reporter assay discriminates nonlipogenic peroxisome proliferator-activated receptor γ ligands
AUTHOR(S): Rival, Yves; Stennevin, Aline; Puech, Laurence; Rouquette, Anne; Cathala, Claudie; Lestienne, Fabrice; Dupont-Passelaigue, Elisabeth; Patoiseau, Jean-Francois; Wurch, Thierry; Junquero, Didier
CORPORATE SOURCE: Centre de Recherche Pierre Fabre, Castres, Fr.
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2004), 311(2), 467-475
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

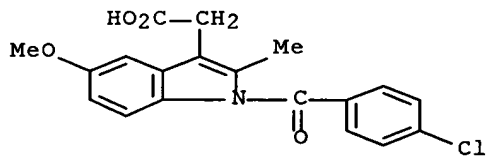
AB Peroxisome proliferator-activated receptors (PPARs) regulate storage and catabolism of fats and carbohydrates. PPARγ activity increases insulin sensitivity and adipocyte differentiation at the expense of adipogenesis and weight gain. The goal of this study was to (1) clone the promoter of the human adipocyte fatty acid binding protein (aP2) gene, namely fatty acid-

binding protein-4, (2) characterize its pharmacol. regulation, and (3) determine its putative predictability for adipogenesis. Among the selected PPAR agonists, rosiglitazone and pioglitazone displayed the highest maximal efficacy (Emax) on reporter-gene assays in COS-7 cells cotransfected by either a galactosidase 4-response element-based or a human aP2 promoter-based Luc reporter vector, along with either chimeric or full-length human PPAR expression plasmids. The non-subtype-selective 2-(4-[2-(3-[2,4-difluorophenyl]-1-heptylureido)ethyl]phenoxy)-2-methyl- butyric acid (GW-2331) and the compds. [4-[3-(4-acetyl-3-hydroxy-2- propylphenoxy)-propoxyl]phenoxy]-acetic acid (L-165041), (4-((2S,5S)-5-(2-(bis(phenylmethyl)amino)-2-oxoethyl)-2-heptyl-4-oxo-3- thiazolidinyl)butyl)-benzoic acid (GW-0072), and indomethacin behaved as partial agonists relative to pioglitazone in full-length human aP2-PPARγ2. Beyond their partial PPARγ agonist properties, these compds. elicited a lower maximal up-regulation of mouse aP2 mRNA in 3T3-L1 adipocytes as compared with pioglitazone; these properties paralleled a time-dependent increase in neutral lipids. By contrast, the selective PPARα agonist 2,2-dichloro-12-(4-chlorophenyl)dodecanoic acid (BM-17.0744) neither stimulated the human aP2-PPARα promoter reporter-gene assay, thus demonstrating a specific interaction between PPARγ and the aP2 promoter, nor affected lipogenesis in 3T3-L1 cells. Altogether, these data characterized a functional promoter of the human aP2 gene; its in vitro pharmacol. regulation in PPARγ-mediated reporter-gene assay may represent an interesting complement or an alternative to time-consuming procedures aiming at discriminating PPAR ligands with low lipogenic properties.

IT 53-86-1, Indomethacin
RL: PAC (Pharmacological activity); BIOL (Biological study)
(human adipocyte fatty acid-binding protein (aP2) gene promoter-driven reporter assay discriminates nonlipogenic peroxisome proliferator-activated receptor γ ligands)

RN 53-86-1 HCAPLUS

CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

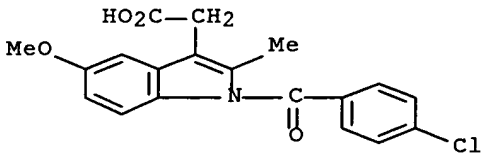
L21 ANSWER 16 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:832890 HCAPLUS Full-text
DOCUMENT NUMBER: 142:19473
TITLE: Comparing Ligand Interactions with Multiple Receptors via Serial Docking
AUTHOR(S): Fernandes, Miguel X.; Kairys, Visvaldas; Gilson, Michael K.
CORPORATE SOURCE: Center for Advanced Research in Biotechnology, U. Maryland Biotechnology Institute, Rockville, MD, 20850, USA
SOURCE: Journal of Chemical Information and Computer Sciences (2004), 44(6), 1961-1970
CODEN: JCISD8; ISSN: 0095-2338

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

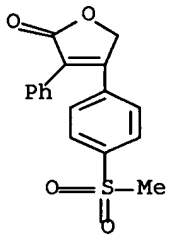
AB Standard uses of ligand-receptor docking typically focus on the association of candidate ligands with a single targeted receptor, but actual applications increasingly require comparisons across multiple receptors. This study demonstrates that comparative docking to multiple receptors can help to select homol. models for virtual compound screening and to discover ligands that bind to one set of receptors but not to another, potentially similar, set. A serial docking algorithm is furthermore described that reduces the computational costs of such calcns. by testing compds. against a series of receptor structures and discarding a compound as soon as it fails to satisfy specified bind/no bind criteria for each receptor. The algorithm also realizes substantial efficiencies by taking advantage of the fact that a ligand typically binds in similar conformations to similar receptors. Thus, once detailed docking has been used to fit a ligand into the first of a series of similar receptors, much less extensive calcns. can be used for the remaining structures.

IT 53-86-1 162011-90-7 169590-42-5
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(ligand interactions with multiple receptors via serial docking through electrostatic force and van der Waals forces)

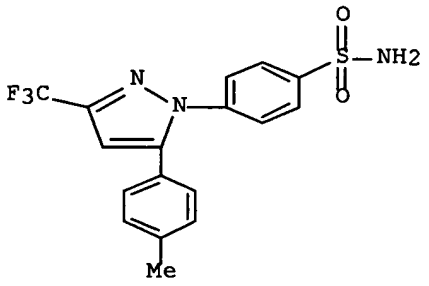
RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



RN 162011-90-7 HCAPLUS
CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 169590-42-5 HCAPLUS
CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 17 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:780365 HCAPLUS Full-text
DOCUMENT NUMBER: 141:295728
TITLE: Preparation of benzene derivatives as cannabinoid receptor ligands
INVENTOR(S): Shankar, Bandarpalle B.; Rizvi, Razia K.; Kozlowski, Joseph A.; Shih, Neng-Yang
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 53 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004186148	A1	20040923	US 2004-803577	20040318
CA 2519401	AA	20041007	CA 2004-2519401	20040318
WO 2004085385	A2	20041007	WO 2004-US8333	20040318
WO 2004085385	A3	20041125		
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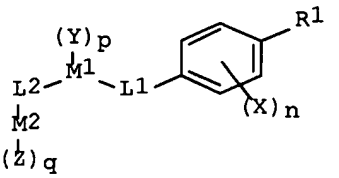
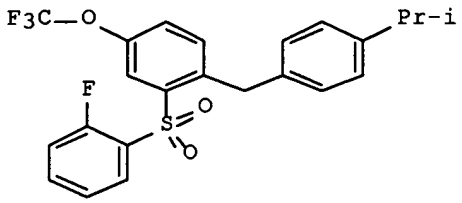
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1611090	A2	20060104	EP 2004-757826	20040318
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1761646	A	20060419	CN 2004-80007295	20040318
PRIORITY APPLN. INFO.:			US 2003-456268P	P 20030320
			WO 2004-US8333	W 20040318

OTHER SOURCE(S): MARPAT 141:295728
GI



I



II

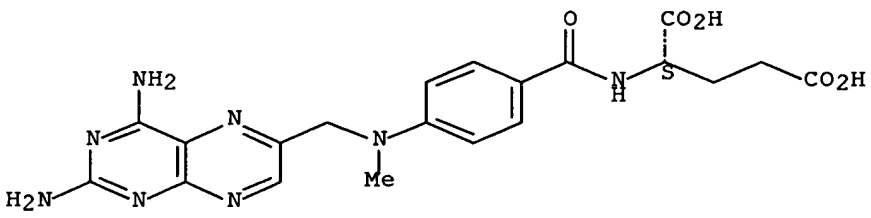
AB Compds. of the formula I [R1 = H, alkoxy, alkyl, aryl, etc.; X = H, alkoxy, cycloalkyl, aryl, etc.; Y = H, OH, CN, alkoxy, alkyl, etc.; Z = H, OH, CN, halo, alkoxy, etc.; L1 = bond, -CF2-, carbonyl, O, S, etc.; L2 = bond, carbonyl, S, SO, SO2, etc.; M1 = aryl cycloalkyl, heteroaryl, heterocycloalkyl; M2 = alkyl, aryl, cycloalkyl, heteroaryl, etc.; n = 0-4; p = 0-4; q = 0-5; with provisions] and the pharmaceutically acceptable salt or solvates thereof, are prepared and disclosed as possessing anti-inflammatory and immunomodulatory activity. Thus, e.g., II was prepared via addition of 4-isopropylphenyllithium (in situ generation from the aryl bromide) to 2-(2-fluorobenzyl)-4-trifluorobenzaldehyde, with subsequent reductive dehydroxylation and sulfur dioxidn. In cannabinoid receptor assays, I demonstrated Ki values ranging from 0.1 nM to 1000 nM. Also disclosed are pharmaceutical compns. containing said compds.

IT 59-05-2, Methotrexate 599-79-1, Sulfasalazine
75706-12-6, Leflunomide 83881-52-1, Zyrtec
153439-40-8, Allegra 162011-90-7, Vioxx
169590-42-5, Celebrex
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(codrug; preparation of benzene derivs. as cannabinoid receptor ligands with antiinflammatory and immunomodulatory activity)

RN 59-05-2 HCAPLUS

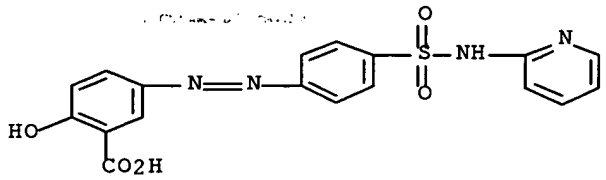
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

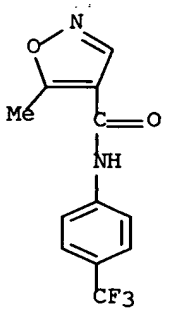


RN 599-79-1 HCAPLUS

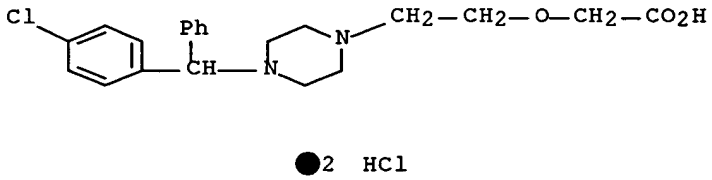
CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)



RN 75706-12-6 HCAPLUS
CN 4-Isoxazolecarboxamide, 5-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

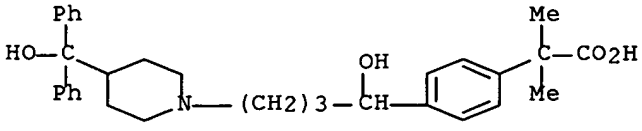


RN 83881-52-1 HCAPLUS
CN Acetic acid, [2-[4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl]ethoxy]-, dihydrochloride (9CI) (CA INDEX NAME)



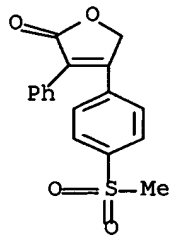
● 2 HCl

RN 153439-40-8 HCAPLUS
CN Benzeneacetic acid, 4-[1-hydroxy-4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]butyl]-α,α-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)

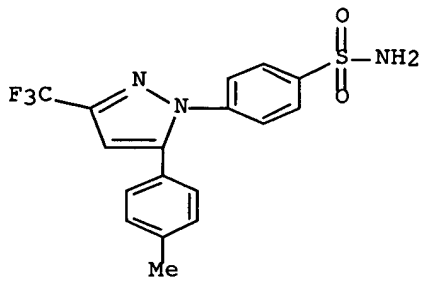


● HCl

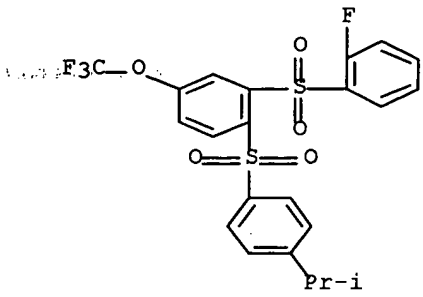
RN 162011-90-7 HCAPLUS
CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



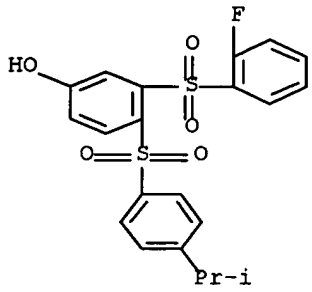
RN 169590-42-5 HCAPLUS
CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



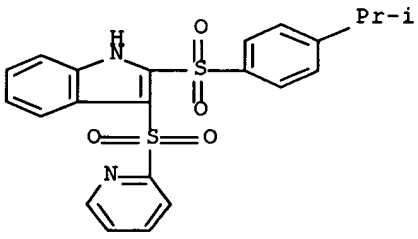
IT 762294-21-3P 762294-23-5P 762294-30-4P
762294-31-5P 762294-33-7P 762294-34-8P
762294-36-0P 762294-38-2P 762294-39-3P
762294-40-6P 762294-41-7P 762294-42-8P
762294-43-9P 762294-44-0P 762294-45-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of benzene derivs. as cannabinoid receptor ligands with antiinflammatory and immunomodulatory activity)
RN 762294-21-3 HCAPLUS
CN Benzene, 2-[(2-fluorophenyl)sulfonyl]-1-[[4-(1-methylethyl)phenyl]sulfonyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



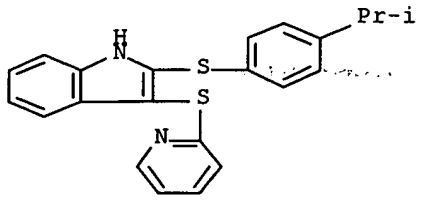
RN 762294-23-5 HCAPLUS
CN Phenol, 3-[(2-fluorophenyl)sulfonyl]-4-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



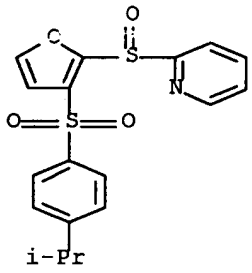
RN 762294-30-4 HCAPLUS
CN 1H-Indole, 2-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



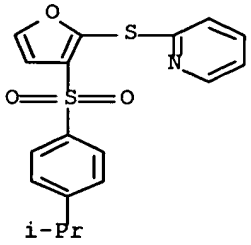
RN 762294-31-5 HCAPLUS
CN 1H-Indole, 2-[[4-(1-methylethyl)phenyl]thio]-3-(2-pyridinylthio)- (9CI) (CA INDEX NAME)



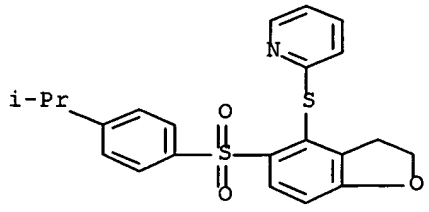
RN 762294-33-7 HCAPLUS
CN Pyridine, 2-[[3-[[4-(1-methylethyl)phenyl]sulfonyl]-2-furanyl]sulfinyl]- (9CI) (CA INDEX NAME)



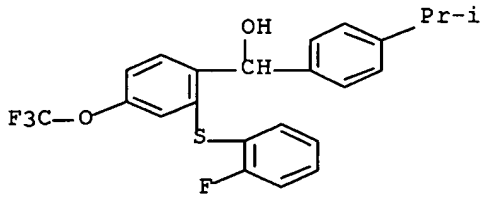
RN 762294-34-8 HCAPLUS
CN Pyridine, 2-[[3-[[4-(1-methylethyl)phenyl]sulfonyl]-2-furanyl]thio]- (9CI) (CA INDEX NAME)



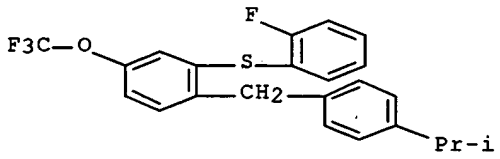
RN 762294-36-0 HCAPLUS
CN Pyridine, 2-[[2,3-dihydro-5-[[4-(1-methylethyl)phenyl]sulfonyl]-4-benzofuranyl]thio]- (9CI) (CA INDEX NAME)



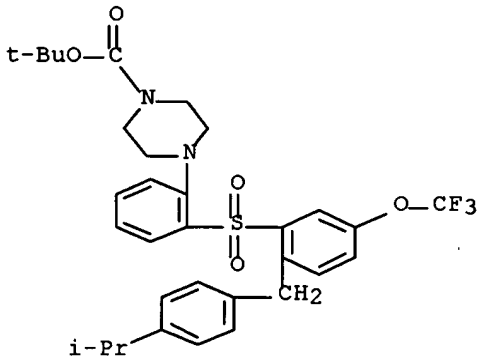
RN 762294-38-2 HCAPLUS
CN Benzenemethanol, 2-[(2-fluorophenyl)thio]-α-[4-(1-methylethyl)phenyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



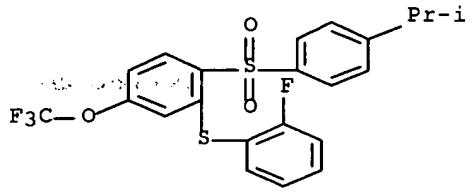
RN 762294-39-3 HCAPLUS
CN Benzene, 2-[(2-fluorophenyl)thio]-1-[[4-(1-methylethyl)phenyl]methyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



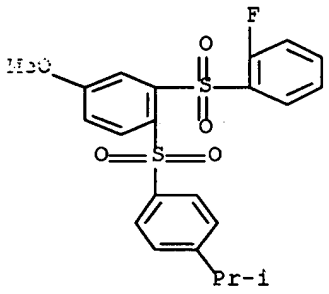
RN 762294-40-6 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[[2-[[4-(1-methylethyl)phenyl]methyl]-5-(trifluoromethoxy)phenyl]sulfonyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



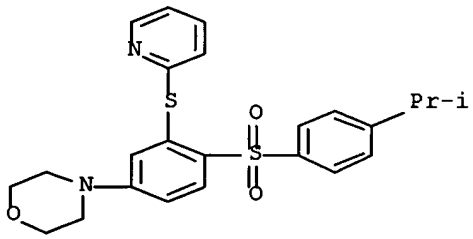
RN 762294-41-7 HCAPLUS
CN Benzene, 2-[(2-fluorophenyl)thio]-1-[[4-(1-methylethyl)phenyl]sulfonyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



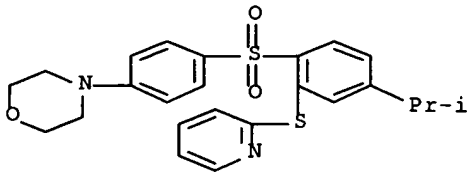
RN 762294-42-8 HCAPLUS
CN Benzene, 2-[(2-fluorophenyl)sulfonyl]-4-methoxy-1-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



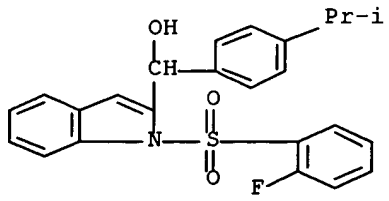
RN 762294-43-9 HCAPLUS
CN Morpholine, 4-[4-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)



RN 762294-44-0 HCAPLUS
CN Morpholine, 4-[4-[[4-(1-methylethyl)-2-(2-pyridinylthio)phenyl]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)



RN 762294-45-1 HCAPLUS
CN 1H-Indole-2-methanol, 1-[(2-fluorophenyl)sulfonyl]-α-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



IT 762294-16-6P 762294-17-7P 762294-18-8P
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762294-27-9P 762294-28-0P 762294-29-1P
762294-32-6P 762294-35-9P 762294-37-1P
762294-46-2P 762294-47-3P 762294-48-4P
762294-49-5P 762294-50-8P 762294-51-9P
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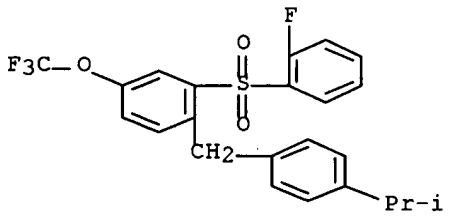
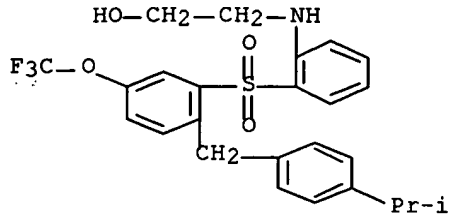
762294-67-7P 762294-68-8P 762294-69-9P
762294-70-2P 762294-71-3P 762294-72-4P
762294-73-5P 762294-74-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzene derivs. as cannabinoid receptor ligands with antiinflammatory and immunomodulatory activity)

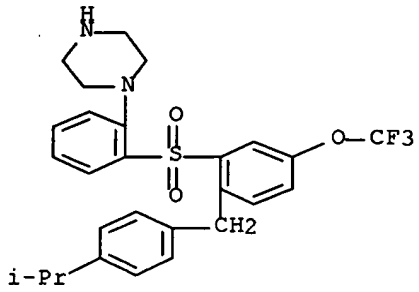
RN 762294-16-6 HCAPLUS
CN Benzene, 2-[(2-fluorophenyl)sulfonyl]-1-[[4-(1-methylethyl)phenyl]methyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



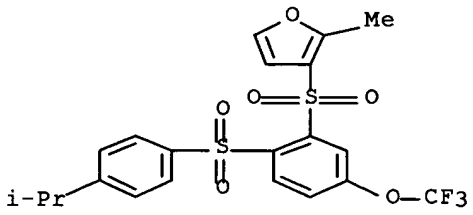
RN 762294-17-7 HCAPLUS
CN Ethanol, 2-[[2-[[2-[[4-(1-methylethyl)phenyl]methyl]-5-(trifluoromethoxy)phenyl]sulfonyl]phenyl]amino]- (9CI) (CA INDEX NAME)



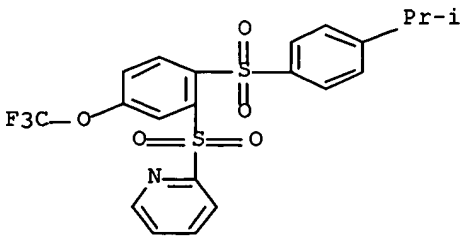
RN 762294-18-8 HCAPLUS
CN Piperazine, 1-[2-[[2-[[4-(1-methylethyl)phenyl]methyl]-5-(trifluoromethoxy)phenyl]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)



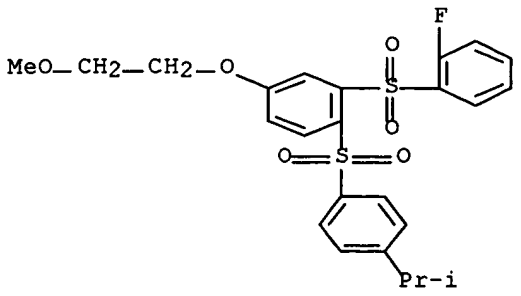
RN 762294-19-9 HCAPLUS
CN Furan, 2-methyl-3-[[2-[[4-(1-methylethyl)phenyl]sulfonyl]-5-(trifluoromethoxy)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



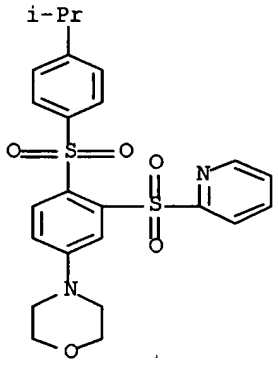
RN 762294-20-2 HCAPLUS
CN Pyridine, 2-[[2-[[4-(1-methylethyl)phenyl]sulfonyl]-5-(trifluoromethoxy)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



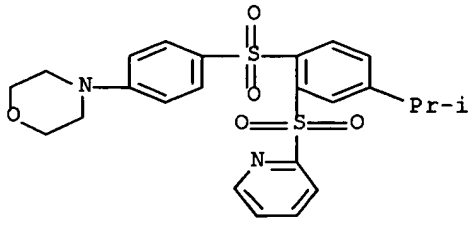
RN 762294-22-4 HCAPLUS
CN Benzene, 2-[(2-fluorophenyl)sulfonyl]-4-(2-methoxyethoxy)-1-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 762294-24-6 HCAPLUS
CN Morpholine, 4-[4-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

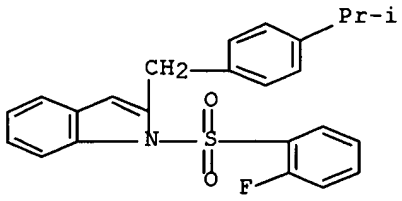


RN 762294-25-7 HCAPLUS
CN Morpholine, 4-[4-[[4-(1-methylethyl)-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

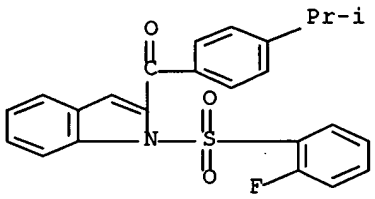


RN 762294-26-8 HCAPLUS
CN 1H-Indole, 1-[(2-fluorophenyl)sulfonyl]-2-[[4-(1-

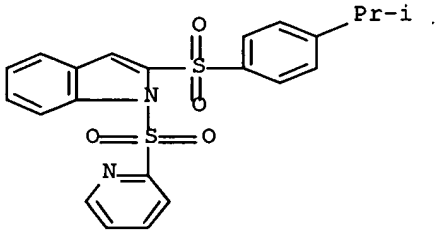
methylethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



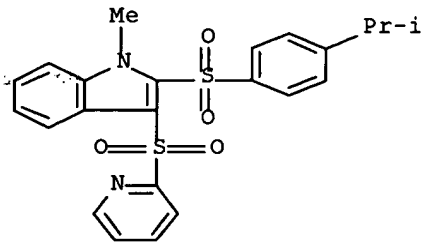
RN 762294-27-9 HCAPLUS
CN 1H-Indole, 1-[(2-fluorophenyl)sulfonyl]-2-[4-(1-methylethyl)benzoyl]- (9CI) (CA INDEX NAME)



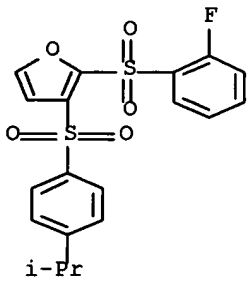
RN 762294-28-0 HCAPLUS
CN 1H-Indole, 2-[[4-(1-methylethyl)phenyl]sulfonyl]-1-(2-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



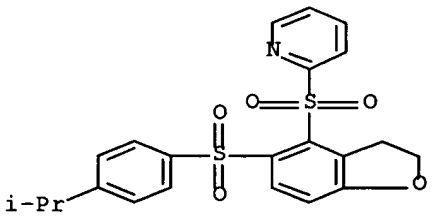
RN 762294-29-1 HCAPLUS
CN 1H-Indole, 1-methyl-2-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



RN 762294-32-6 HCAPLUS
CN Furan, 2-[(2-fluorophenyl)sulfonyl]-3-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

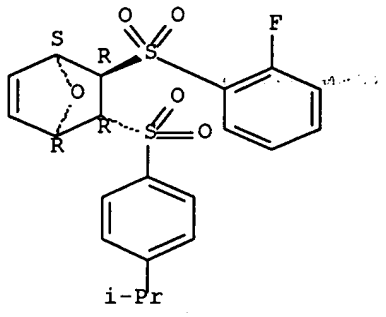


RN 762294-35-9 HCAPLUS
CN Pyridine, 2-[[2,3-dihydro-5-[[4-(1-methylethyl)phenyl]sulfonyl]-4-benzofuranyl]sulfonyl]- (9CI) (CA INDEX NAME)

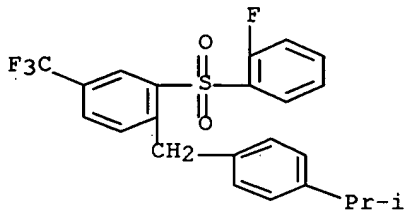


RN 762294-37-1 HCAPLUS
CN 7-Oxabicyclo[2.2.1]hept-2-ene, 5-[(2-fluorophenyl)sulfonyl]-6-[[4-(1-methylethyl)phenyl]sulfonyl]-, (1R,4S,5R,6R)-rel- (9CI) (CA INDEX NAME)

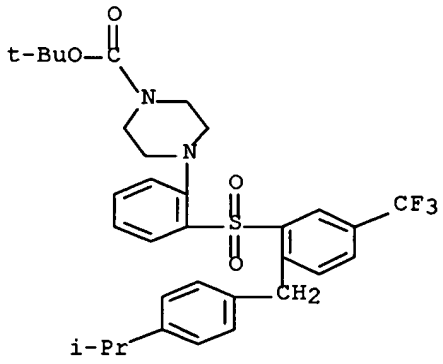
Relative stereochemistry.



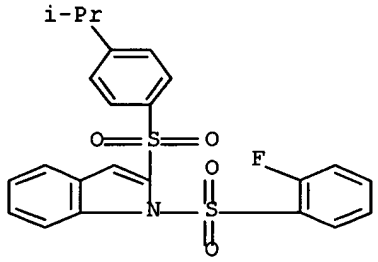
RN 762294-46-2 HCAPLUS
CN Benzene, 2-[(2-fluorophenyl)sulfonyl]-1-[[4-(1-methylethyl)phenyl]methyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



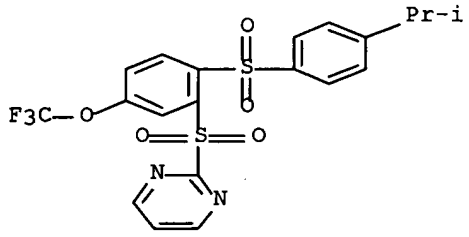
RN 762294-47-3 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[[2-[[4-(1-methylethyl)phenyl]methyl]-5-(trifluoromethyl)phenyl]sulfonyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



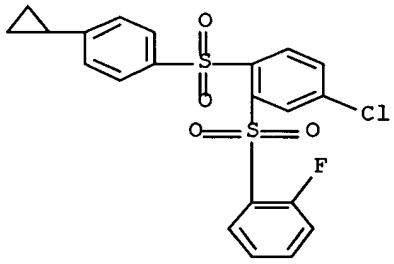
RN 762294-48-4 HCAPLUS
CN 1H-Indole, 1-[(2-fluorophenyl)sulfonyl]-2-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



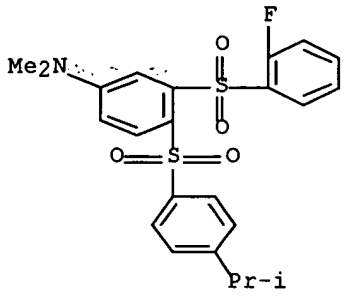
RN 762294-49-5 HCAPLUS
CN Pyrimidine, 2-[[2-[[4-(1-methylethyl)phenyl]sulfonyl]-5-(trifluoromethoxy)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



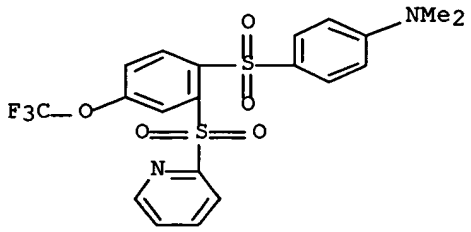
RN 762294-50-8 HCAPLUS
CN Benzene, 4-chloro-1-[(4-cyclopropylphenyl)sulfonyl]-2-[(2-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)



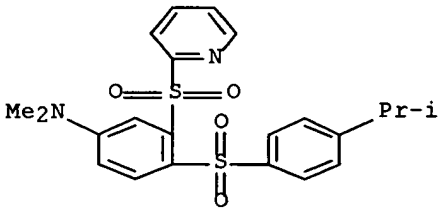
RN 762294-51-9 HCAPLUS
CN Benzenamine, 3-[(2-fluorophenyl)sulfonyl]-N,N-dimethyl-4-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



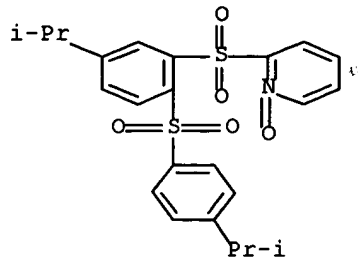
RN 762294-52-0 HCAPLUS
CN Benzenamine, N,N-dimethyl-4-[[2-(2-pyridinylsulfonyl)-4-(trifluoromethoxy)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



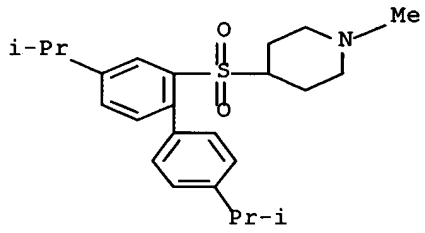
RN 762294-53-1 HCAPLUS
CN Benzenamine, N,N-dimethyl-4-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



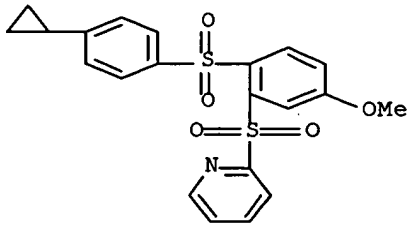
RN 762294-54-2 HCAPLUS
CN Pyridine, 2-[[5-(1-methylethyl)-2-[[4-(1-methylethyl)phenyl]sulfonyl]phenyl]sulfonyl]-, 1-oxide (9CI) (CA INDEX NAME)



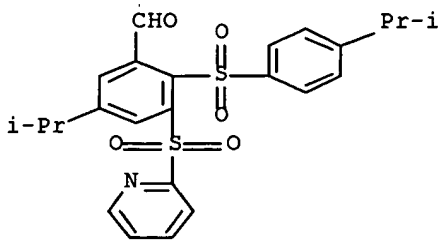
RN 762294-55-3 HCAPLUS
CN Piperidine, 4-[[4,4'-bis(1-methylethyl)[1,1'-biphenyl]-2-yl]sulfonyl]-1-methyl- (9CI) (CA INDEX NAME)



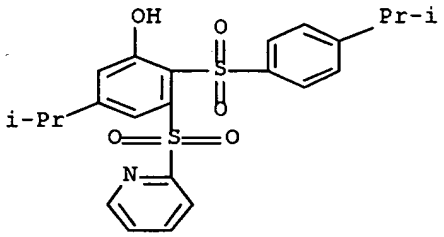
RN 762294-56-4 HCAPLUS
CN Pyridine, 2-[[2-[(4-cyclopropylphenyl)sulfonyl]-5-methoxyphenyl]sulfonyl]- (9CI) (CA INDEX NAME)



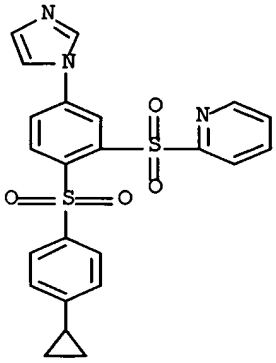
RN 762294-57-5 HCAPLUS
CN Benzaldehyde, 5-(1-methylethyl)-2-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



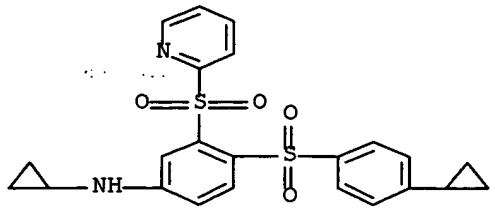
RN 762294-58-6 HCAPLUS
CN Phenol, 5-(1-methylethyl)-2-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



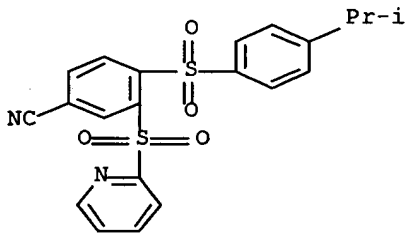
RN 762294-59-7 HCAPLUS
CN Pyridine, 2-[[2-[(4-cyclopropylphenyl)sulfonyl]-5-(1H-imidazol-1-yl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



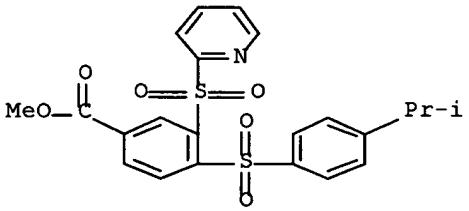
RN 762294-60-0 HCAPLUS
CN Benzenamine, N-cyclopropyl-4-[(4-cyclopropylphenyl)sulfonyl]-3-(2-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



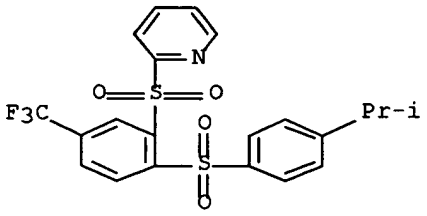
RN 762294-61-1 HCAPLUS
CN Benzonitrile, 4-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylsulfonyl)- (9CI) (CA INDEX NAME)



RN 762294-62-2 HCAPLUS
CN Benzoic acid, 4-[[4-(1-methylethyl)phenyl]sulfonyl]-3-(2-pyridinylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

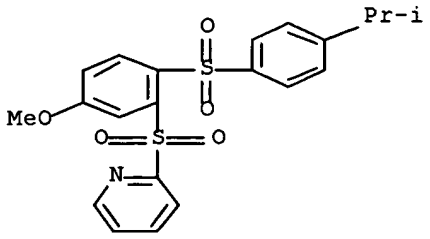


RN 762294-63-3 HCAPLUS
CN Pyridine, 2-[[2-[[4-(1-methylethyl)phenyl]sulfonyl]-5-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



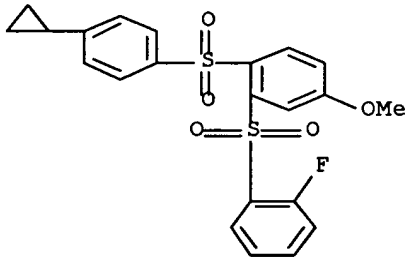
RN 762294-64-4 HCAPLUS

CN Pyridine, 2-[[5-methoxy-2-[[4-(1-methylethyl)phenyl]sulfonyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



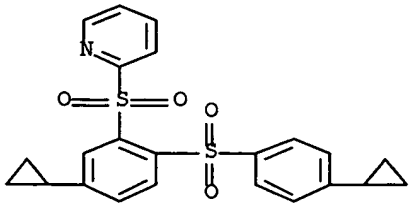
RN 762294-65-5 HCAPLUS

CN Benzene, 1-[(4-cyclopropylphenyl)sulfonyl]-2-[(2-fluorophenyl)sulfonyl]-4-methoxy- (9CI) (CA INDEX NAME)



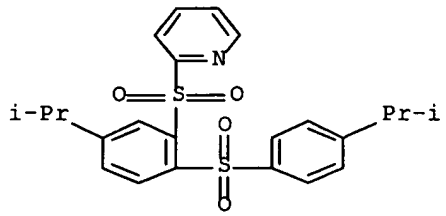
RN 762294-66-6 HCAPLUS

CN Pyridine, 2-[[5-cyclopropyl-2-[(4-cyclopropylphenyl)sulfonyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

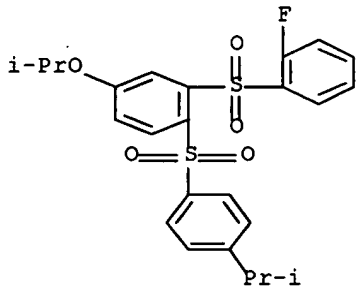


RN 762294-67-7 HCAPLUS

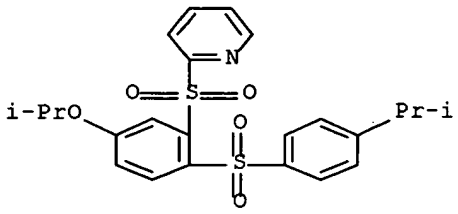
CN Pyridine, 2-[[5-(1-methylethyl)-2-[[4-(1-methylethyl)phenyl]sulfonyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



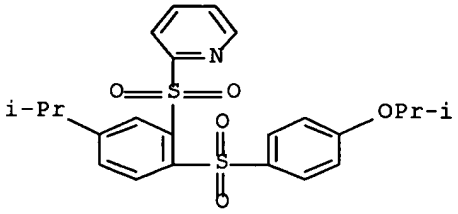
RN 762294-68-8 HCAPLUS
CN Benzene, 2-[(2-fluorophenyl)sulfonyl]-4-(1-methylethoxy)-1-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



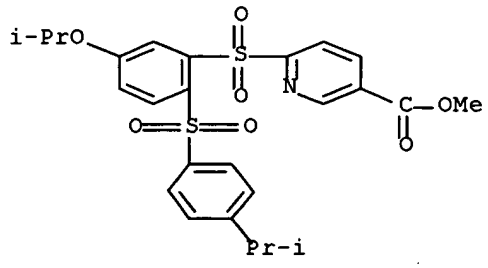
RN 762294-69-9 HCAPLUS
CN Pyridine, 2-[[5-(1-methylethoxy)-2-[[4-(1-methylethyl)phenyl]sulfonyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



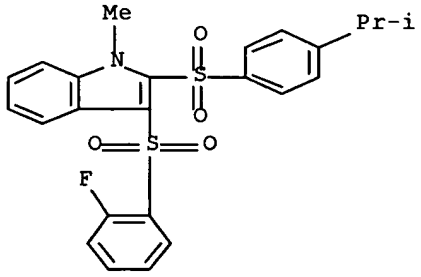
RN 762294-70-2 HCAPLUS
CN Pyridine, 2-[[2-[[4-(1-methylethoxy)phenyl]sulfonyl]-5-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



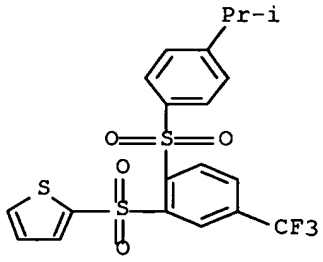
RN 762294-71-3 HCAPLUS
CN 3-Pyridinecarboxylic acid, 6-[[5-(1-methylethoxy)-2-[[4-(1-methylethyl)phenyl]sulfonyl]phenyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)



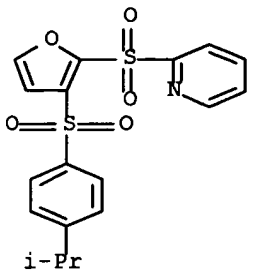
RN 762294-72-4 HCAPLUS
CN 1H-Indole, 3-[(2-fluorophenyl)sulfonyl]-1-methyl-2-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 762294-73-5 HCAPLUS
CN Thiophene, 2-[[2-[[4-(1-methylethyl)phenyl]sulfonyl]-5-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

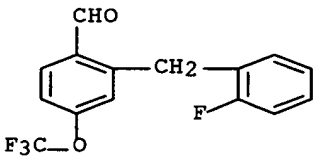


RN 762294-74-6 HCAPLUS
CN Pyridine, 2-[[3-[[4-(1-methylethyl)phenyl]sulfonyl]-2-furanyl]sulfonyl]- (9CI) (CA INDEX NAME)

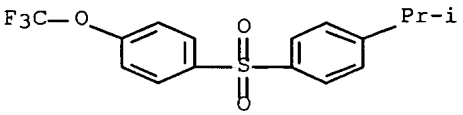


IT 762294-75-7P 762294-77-9P 762294-78-0P
762294-79-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzene derivs. as cannabinoid receptor ligands with antiinflammatory and immunomodulatory activity)

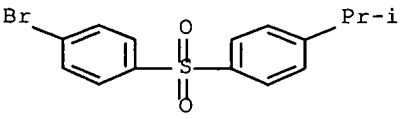
RN 762294-75-7 HCAPLUS
CN Benzaldehyde, 2-[(2-fluorophenyl)methyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



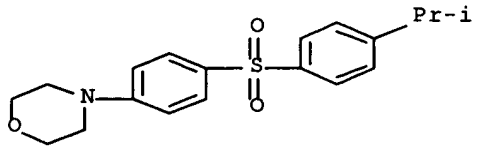
RN 762294-77-9 HCAPLUS
CN Benzene, 1-[[4-(1-methylethyl)phenyl]sulfonyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



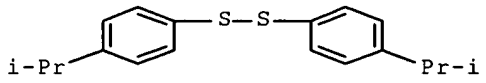
RN 762294-78-0 HCAPLUS
CN Benzene, 1-bromo-4-[[4-(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 762294-79-1 HCAPLUS
CN Morpholine, 4-[4-[[4-(1-methylethyl)phenyl]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)



IT 622407-64-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzene derivs. as cannabinoid receptor ligands with antiinflammatory and immunomodulatory activity)
RN 622407-64-1 HCAPLUS
CN Disulfide, bis[4-(1-methylethyl)phenyl] (9CI) (CA INDEX NAME)



L21 ANSWER 18 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:701965 HCAPLUS Full-text
DOCUMENT NUMBER: 141:218942
TITLE: Use of ligands for the guanylyl cyclase receptor for heat-stable enterotoxin in the treatment of colorectal, gastric and esophageal cancer
INVENTOR(S): Waldman, Scott A.; Pitari, Giovanni Mario; Park, Jason; Schulz, Stephanie; Wolfe, Henry R.
PATENT ASSIGNEE(S): Thomas Jefferson University, USA
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004071436	A2	20040826	WO 2004-US3765	20040210
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004258687	A1	20041223	US 2004-775481	20040210
EP 1599165	A2	20051130	EP 2004-709828	20040210
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRIORITY APPLN. INFO.: US 2003-446730P P 20030210
WO 2004-US3765 W 20040210

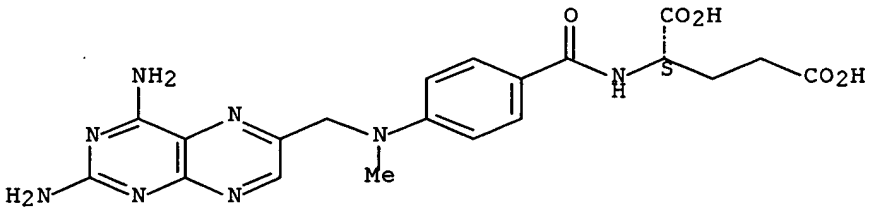
AB Methods of inhibiting the proliferation of colorectal, gastric and esophageal cancer cells in the treatment of the disease is described. The target for the inhibition of cell proliferation is guanylyl cyclease C, the receptor for heat-stable enterotoxin ST. The therapeutic ligand may be heat-stable enterotoxin ST or peptides derived from it. The enzyme may also be a target in the treatment of metastasized colorectal or primary or metastatic gastric or esophageal cancer. Methods of increasing the number of ST receptor mols. on the surface of a colorectal cell, including in colorectal cancer by administration of ligands for the receptor are disclosed. The presence of the receptor to image tumors in the diagnosis of primary or metastatic colorectal cancer are also described. Methods of delivering an active compound to a colorectal cell in an individual are disclosed. Epidemiol. studies show that the incidence of colorectal cancer falls with increasing incidence of enterotoxigenic Escherichia coli. DNA synthesis is inhibited by ST enterotoxin in cells presenting guanylyl cyclase C by the action of the toxin on cyclic nucleotide-gated calcium channels. The enterotoxin also inhibits the release of matrix metalloproteinase 9, which plays a role in the release of cancer cells from the extracellular matrix and in metastasis, by preventing organization of the actin cytoskeleton.

IT 59-05-2, Methotrexate
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cancer therapy with enterotoxin ST peptides and; use of ligands for guanylyl cyclase receptor for heat-stable enterotoxin in treatment of colorectal, gastric and esophageal cancer)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 19 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:510777 HCAPLUS Full-text
DOCUMENT NUMBER: 141:47307
TITLE: Saposin c and receptors as targets for treatment of benign and malignant disorders
INVENTOR(S): Koochekpour, Shahriar; Sartor, A. Oliver
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 31 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 2004120961	A1	20040624	US 2002-324993	20021220
CA 2510313	AA	20040715	CA 2003-2510313	20031218
WO 2004058165	A2	20040715	WO 2003-US40648	20031218
WO 2004058165	A3	20050324		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003301135	A1	20040722	AU 2003-301135	20031218
EP 1578436	A2	20050928	EP 2003-814232	20031218

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:

US 2002-324993	A	20021220
WO 2003-US40648	W	20031218

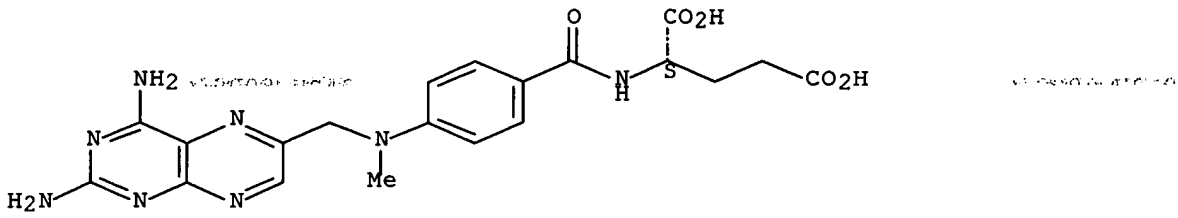
AB Saposin C was shown to be a trophic factor for a variety of cancer cells, e.g., prostate, lung, breast, and colon cancer cells. These cells expressed saposin C and responded to saposin C by increased levels of cell proliferation, cell migration, and cell invasion. Such activities typify and promote the neoplastic process. For prostate cancer, the androgen-insensitive prostate cancer cells responded to saposin C by higher levels of cell proliferation, cell migration and cell invasion than did the androgen-sensitive prostate cells. Stromal cells (from the prostate) were also responsive to saposin C-mediated signals in a manner typical of growth promoting compds. The androgen-insensitive prostate cells were stimulated by saposin C to express higher levels of the urokinase plasminogen activator (uPA) and its receptor (uPAR), two proteins known to be involved in cell invasion. A conjugate of a peptide of the active region of saposin C (TX14A) and a toxin (saporin) was made and was shown to decrease the survival of prostate cancer cells, and the other cancer cells that were found to express saposin C (including cancers cells of the breast, colon, and lung). This conjugate or a compound of analogous action that inhibits cellular growth acting via a saposin-C binding receptor can be used to decrease tumor growth and/or treat disorders of stromal proliferation (e.g., benign prostatic hyperplasia, atherosclerosis, and vascular restenosis).

IT 59-05-2D, Methotrexate, conjugates with ligands
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(saposin c and receptors as targets for treatment of benign and malignant disorders)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

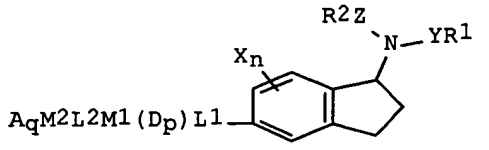
Absolute stereochemistry.



L21 ANSWER 20 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:467852 HCAPLUS Full-text
DOCUMENT NUMBER: 141:38447
TITLE: Preparation of indanesulfonamides and related compounds as cannabinoid CB2 receptor ligands
INVENTOR(S): Tong, Ling; Chen, Lei; Shankar, Bandarpalle B.; Kozlowski, Joseph A.; Shih, Neng-Yang
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004048322	A1	20040610	WO 2003-US37366	20031121
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2506895	AA	20040610	CA 2003-2506895	20031121
AU 2003294449	A1	20040618	AU 2003-294449	20031121
US 2004132804	A1	20040708	US 2003-721015	20031121
EP 1565431	A1	20050824	EP 2003-789933	20031121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1741992	A	20060301	CN 2003-80109091	20031121
JP 2006507347	T2	20060302	JP 2004-555591	20031121
PRIORITY APPLN. INFO.:			US 2002-428861P P	20021125
			WO 2003-US37366 W	20031121

OTHER SOURCE(S): MARPAT 141:38447
GI



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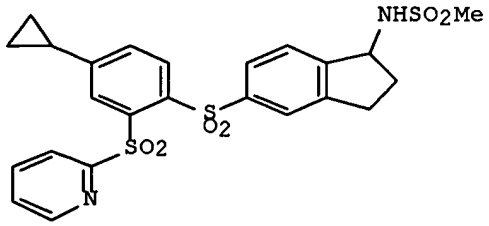


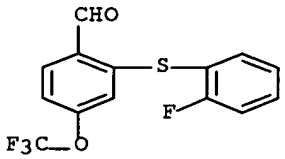
II

AB Title compds. [I; R1, R2 = H, CF3, (substituted) alkyl, alkoxy, cycloalkyl, heterocycloalkyl, heteroaryl, etc.; R1YNZR2 = atoms to form a 4-8 membered (substituted) heterocycloalkyl; X = alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; L1 = C(R2)2, O2C, CO, S, SO2, SO, NHCO, etc.; L2 = bond, C(R2)2, S, SO, SO2, O, N(R2)2, CONH, CF2, etc.; M1 = (substituted) aryl, heteroaryl, cycloalkyl, heterocycloalkyl; M2 = (substituted) alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl; n = 0-3; p = 0-4; q = 0-5], were prepared Thus, title compound (II) (multistep preparation from 5-bromo-1-indanone given) showed CB2 inhibitory activity with Ki <20 nM.

IT 447460-19-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indanesulfonamides and related compds. as cannabinoid CB2 receptor ligands)

RN 447460-19-7 HCAPLUS

CN Benzaldehyde, 2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



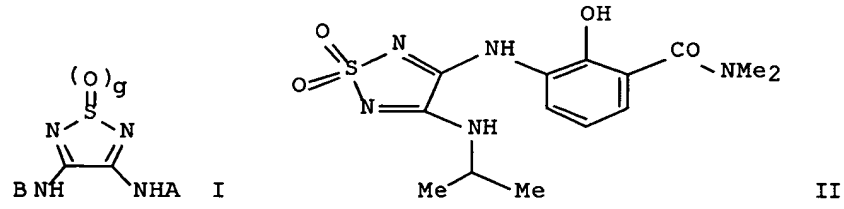
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 21 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:333705 HCAPLUS Full-text
DOCUMENT NUMBER: 140:357355
TITLE: Preparation of diaminothiadiazole dioxides and monoxides as CXC- and CC-chemokine receptor ligands
INVENTOR(S): Taveras, Arthur G.; Chao, Jianhua; Biju, Purakkattle J.; Yu, Younong; Fine, Jay S.; Hipkin, William; Aki, Cynthia J.; Merritt, J. Robert; Li, Ge; Baldwin, John J.; Lai, Gaifa; Wu, Minglang; Hecker, Evan A.
PATENT ASSIGNEE(S): Pharmacopeia, Inc., USA; Schering Corporation; Pharmacopeia Drug Discovery, Inc.

SOURCE: PCT Int. Appl., 540 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004033440	A1	20040422	WO 2003-US31707	20031007
WO 2004033440	C1	20050602		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, [illegible], ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2501535	AA	20040422	CA 2003-2501535	20031007
AU 2003288922	A1	20040504	AU 2003-288922	20031007
US 2004186142	A1	20040923	US 2003-680393	20031007
EP 1551818	A1	20050713	EP 2003-781311	20031007
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1720240	A	20060111	CN 2003-80105139	20031007
JP 2006508079	T2	20060309	JP 2004-543449	20031007
PRIORITY APPLN. INFO.:			US 2002-417371P	P 20021009
			WO 2003-US31707	W 20031007

OTHER SOURCE(S): MARPAT 140:357355
GI



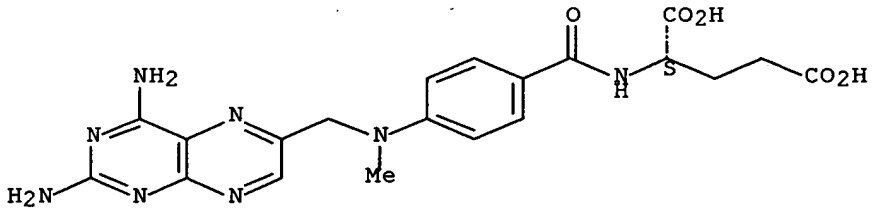
AB Disclosed are diaminothiadiazole mono- and dioxides (shown as I; e.g. II) and the pharmaceutically acceptable salts and solvates thereof. Examples of substituent A include heteroaryl, aryl, heterocycloalkyl, cycloalkyl, aryl, alkynyl, alkenyl, aminoalkyl, alkyl or amino; examples of substituent B include aryl and heteroaryl; g = 1, 2. Also disclosed is a method of treating a chemokine mediated diseases, such as, cancer, angiogenesis, angiogenic ocular diseases, pulmonary diseases, multiple sclerosis, rheumatoid arthritis, osteoarthritis, stroke and cardiac reperfusion injury, acute pain, acute and chronic inflammatory pain, and neuropathic pain using I. Although the methods of preparation are not claimed, hundreds of example prepns. and/or characterization data are included. For example, II was prepared in 31% yield

from the 4-methoxy analog and isopropylamine in the presence of DIEA in MeOH; the 4-methoxy analog was prepared from the dimethoxy analog and N,N-dimethyl-3-amino-2- hydroxybenzamide in 99% crude yield. Antagonist activities of some examples of I towards CXCR1, CXCR2 and CCR7 are given.

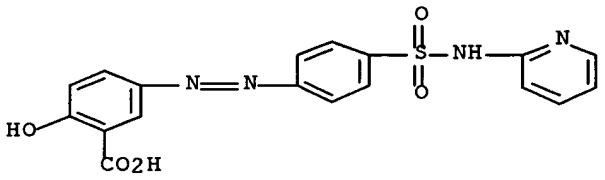
IT 59-05-2, Methotrexate 599-79-1, Sulfasalazine
75706-12-6, Leflunomide
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(codrug for multiple sclerosis; preparation of diaminothiadiazole dioxides and monoxides as CXC- and CC-chemokine receptor ligands)

RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

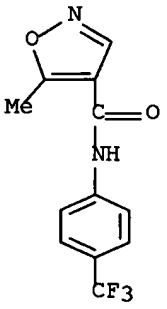
Absolute stereochemistry.



RN 599-79-1 HCAPLUS
CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)



RN 75706-12-6 HCAPLUS
CN 4-Isoxazolecarboxamide, 5-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 22 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:20974 HCAPLUS Full-text
DOCUMENT NUMBER: 140:71069
TITLE: Methods and compositions using hyaluronan receptor ligands for inhibition of multidrug resistance
INVENTOR(S): Toole, Bryan P.
PATENT ASSIGNEE(S): Tufts University, USA
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004003545	A1	20040108	WO 2003-US20918	20030701
WO 2004003545	C2	20040415		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2513143	AA	20040108	CA 2003-2513143	20030701
AU 2003280471	A1	20040119	AU 2003-280471	20030701
EP 1532434	A1	20050525	EP 2003-742415	20030701
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005532373	T2	20051027	JP 2004-518221	20030701
US 2004229843	A1	20041118	US 2004-835511	20040429

PRIORITY APPLN. INFO.:

US 2002-392905P	P	20020701
US 2003-453761P	P	20030311
WO 2003-US20918	W	20030701

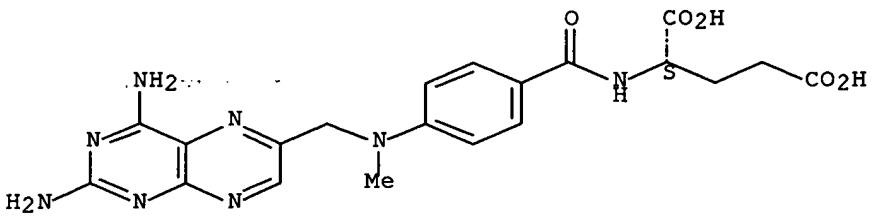
AB Pharmaceutical compns. and methods are provided for sensitizing multidrug-resistant cancer or radiation-resistant cancer cells to chemotherapeutic agents. Compns. include ligands of hyaluronan receptors, including glycosaminoglycans, e.g. hyaluronan oligomers and derivs. of these oligomers, hyaluronan binding proteins, and antibodies specific for hyaluronan receptors. The multidrug-resistance cells may also be bacterial cells.

IT 59-05-2, Methotrexate
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hyaluronan receptor ligands for inhibition of multidrug resistance)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 23 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:991368 HCAPLUS Full-text
DOCUMENT NUMBER: 140:35953
TITLE: Compositions and methods for treating diabetes via pancreatic islet neogenesis
INVENTOR(S): Brand, Stephen J.; Cruz, Antonio
PATENT ASSIGNEE(S): Waratah Pharmaceuticals, Inc., Can.
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003103701	A1	20031218	WO 2003-US18377	20030609
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2486584	AA	20031218	CA 2003-2486584	20030609
AU 2003243501	A1	20031222	AU 2003-243501	20030609
US 2004023885	A1	20040205	US 2003-457126	20030609
EP 1511509	A1	20050309	EP 2003-757483	20030609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671407	A	20050921	CN 2003-818526	20030609
JP 2005533775	T2	20051110	JP 2004-510820	20030609
PRIORITY APPLN. INFO.:			US 2002-387032P	P 20020607
			US 2002-430590P	P 20021203
			US 2002-387032	A 20020607
			US 2002-430590	A 20021203
			WO 2003-US18377	W 20030609

AB Compns. and methods for islet neogenesis therapy comprising an EGF and a gastrin in combination with immune suppression, and for treating or preventing early stage diabetes with a gastrin/CCK receptor ligand and an immunosuppressant are provided.

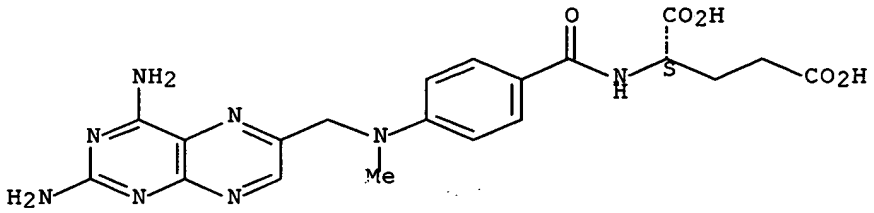
IT 59-05-2, Methotrexate
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)
(compns. and methods for treating diabetes via pancreatic islet neogenesis using immune suppression and gastrin-CCK receptor ligand)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 24 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:991176 HCAPLUS Full-text

DOCUMENT NUMBER: 140:27654

TITLE: Preparation of N-(α-methylbenzyl) sulfonamides as cannabinoid receptor ligands

INVENTOR(S): Kozlowski, Joseph A.; Shih, Neng-Yang; Lavey, Brian J.; Rizvi, Razia K.; Shankar, Bandarpalle B.; Spitler, James M.; Tong, Ling; Wolin, Ronald L.; Wong, Michael K.

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: U.S. Pat. Appl. Publ., 68 pp., Cont.-in-part of U.S. Ser. No. 72,354.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003232859	A1	20031218	US 2002-214897	20020807
US 7067539	B2	20060627		
US 2003096844	A1	20030522	US 2002-72354	20020206
ZA 2003005933	A	20041101	ZA 2003-5933	20030731
CA 2494827	AA	20040219	CA 2003-2494827	20030805
WO 2004014825	A1	20040219	WO 2003-US24398	20030805

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003257172	A1	20040225	AU 2003-257172	20030805
EP 1539662	A1	20050615	EP 2003-784905	20030805
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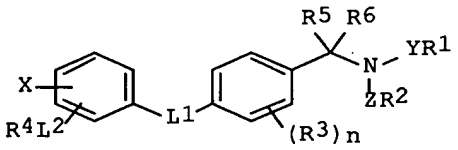
JP 2005534715	T2	20051117	JP 2004-527741	20030805
US 2006009528	A1	20060112	US 2005-203946	20050815
PRIORITY APPLN. INFO.:			US 2001-267375P	P 20010208
			US 2001-292600P	P 20010522
			US 2002-72354	A2 20020206
			US 2002-214897	A 20020807
			WO 2003-US24398	W 20030805

OTHER SOURCE(S): MARPAT 140:27654

GI



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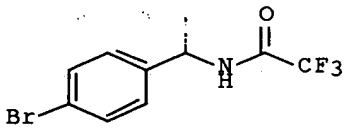

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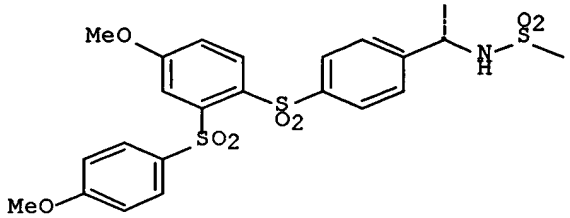


III

AB Title compds. [I; R1 = H, alkyl, haloalkyl, cycloalkyl, cycloalkylamino, aralkyl, heteroaryl, amino, (substituted) aryl, etc.; R2, R5, R6 = H, alkyl; R3 = H, alkyl, Cl, F, CF3, OCF2H, OCF3, OH, alkoxy; R4 = H, (substituted) alkyl, alkoxy, cycloalkyl, alkenyl, aryl, PhCH2, heteroaryl, arylamino, heteroarylamino, cycloalkylamino, etc.; L1 = alkylene, alkenylene, CO, C(R2)2, CHOR2, NOR5, SO2, SO, S, O, NR2, NR2CO, CHCF3, CF2; L2 = bond, alkylene, CO, C(R2)2, NR2, NR2SO2, CONR2, S, SO, SO2, NOR5, CR2OH, etc.; X = H, halo, CF3, cyano, OCF2H, OCF3, alkyl, cycloalkyl, cycloalkoxy, alkoxy, heteroalkyl, CO2R2, NHR2, arylamino, OSO2R2, etc.; Y, Z = bond, CH2, SO2, CO; R1YNZR2 = atoms to form a heterocycle; n = 0-4], were prepared for treatment of cancer, inflammatory disease, immunomodulatory disease, or respiratory disease (no data). Thus, (S)-α-methylbenzylamine was stirred with (F3CCO)2O in CH2Cl2; the mixture was then treated with MeSO3H and dibromodimethylhydantoin to give 32% intermediate (II). II in THF at -78° was treated with MeLi and then with 4-MeOC6H4SO2Cl followed by warming to room temperature to give 65% di-Ph sulfone derivative The latter in THF at -78° was treated with BuLi then with bis(4-methoxyphenyl)disulfide to give crude disulfide coupling product, which was treated with MCPBA in CH2Cl2 to give 45% bissulfone. This was deprotected with LiOH in H2O/dioxane followed by treatment with MeSO2Cl to give title compound (III). Pharmaceutical compns. comprising the compound I are claimed.

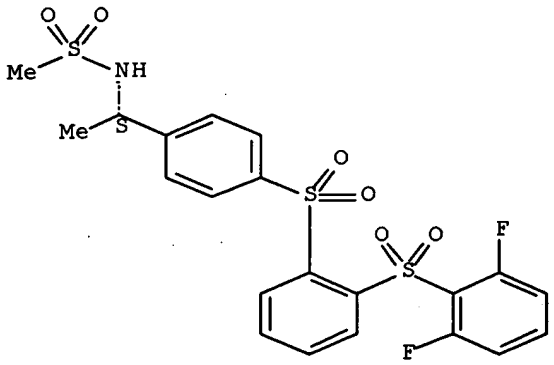
IT 447459-44-1P 447459-45-2P 447459-46-3P
447459-47-4P 447459-48-5P 447459-49-6P
447459-50-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of methylbenzylsulfonamides as cannabinoid receptor ligands)

RN 447459-44-1 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

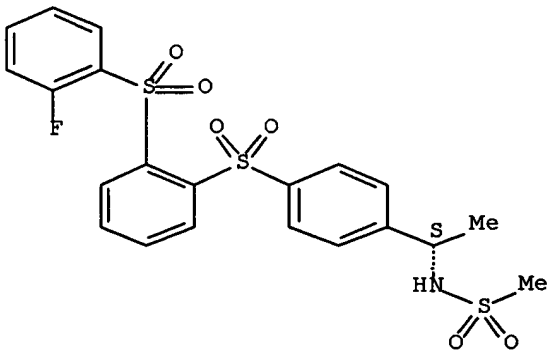
Absolute stereochemistry.



RN 447459-45-2 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

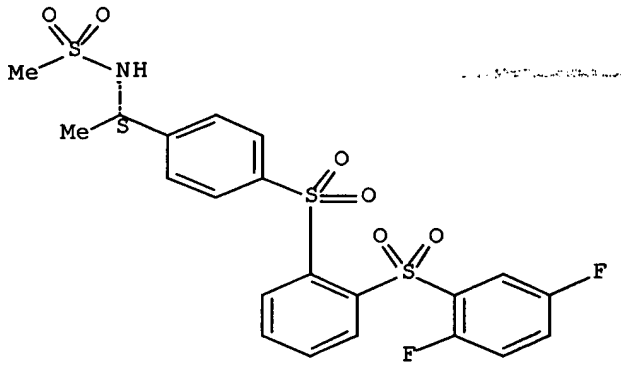
Absolute stereochemistry.



RN 447459-46-3 HCAPLUS

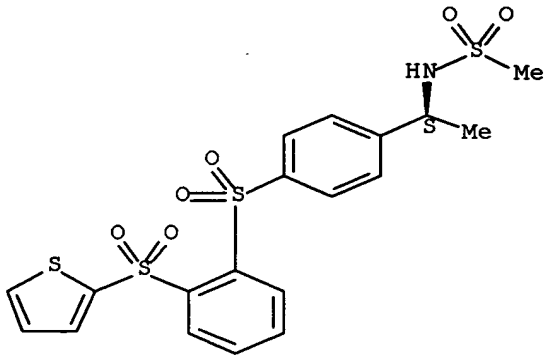
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2,5-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



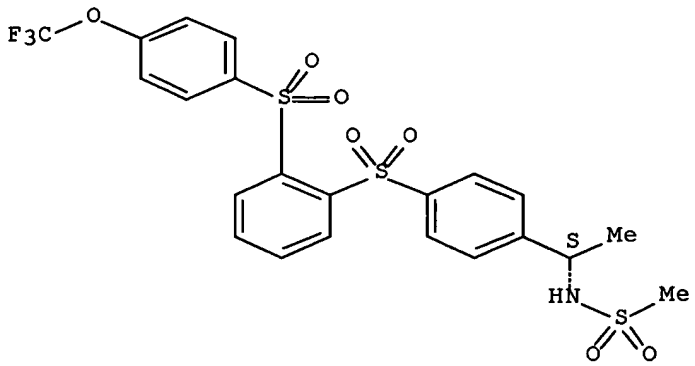
RN 447459-47-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-(2-thienylsulfonyl)phenyl]sulfonyl]ph
enyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



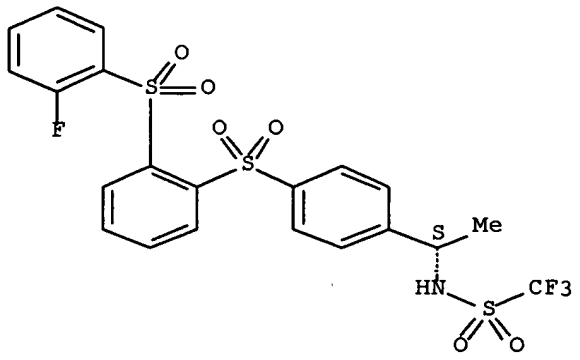
RN 447459-48-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[[4-(trifluoromethoxy)phenyl]sulfonyl
]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



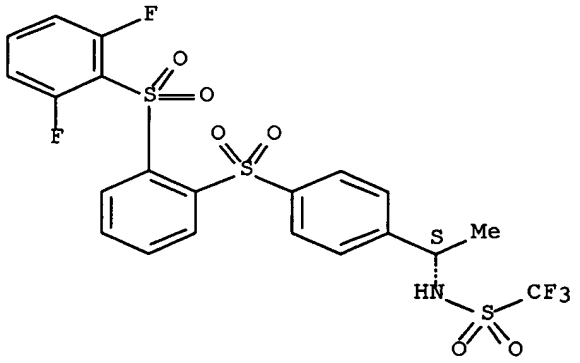
RN 447459-49-6 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



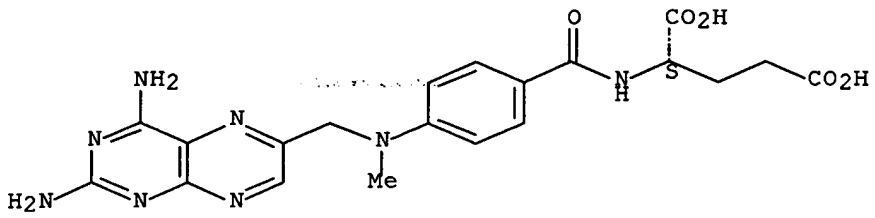
RN 447459-50-9 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

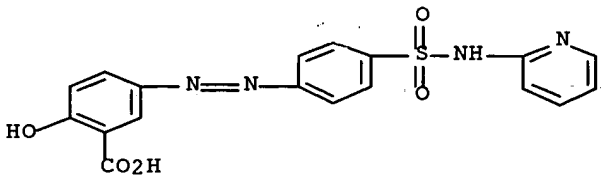


IT 59-05-2, Methotrexate 599-79-1, Sulfasalazine
162011-90-7, Vioxx 169590-42-5, Celebrex
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(co-administration; preparation of methylbenzylsulfonamides as cannabinoid receptor ligands for treating rheumatoid arthritis in combination with other agents)
RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

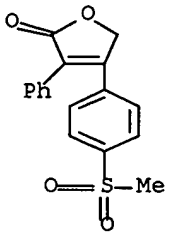
Absolute stereochemistry.



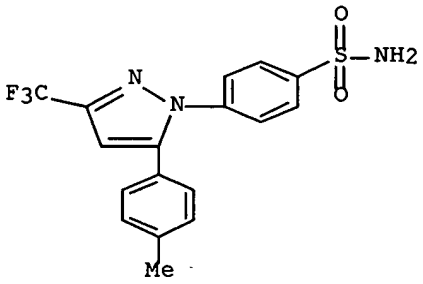
RN 599-79-1 HCAPLUS
CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)



RN 162011-90-7 HCAPLUS
CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 169590-42-5 HCAPLUS
CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



IT 447459-51-0P 447459-52-1P 447459-53-2P
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447459-57-6P 447459-58-7P 447459-59-8P
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447459-79-2P 447459-80-5P 447459-81-6P
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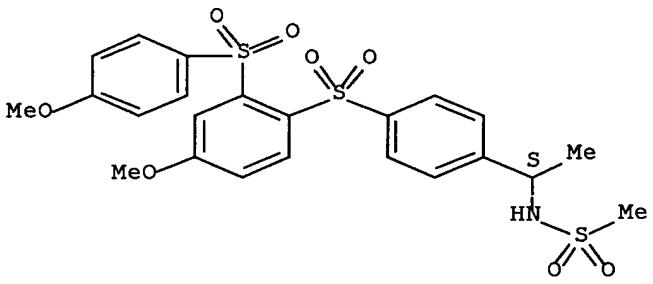
447459-91-8P 447459-92-9P 447459-93-0P
447459-94-1P 447459-95-2P 447459-96-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of methylbenzylsulfonamides as cannabinoid receptor ligands)

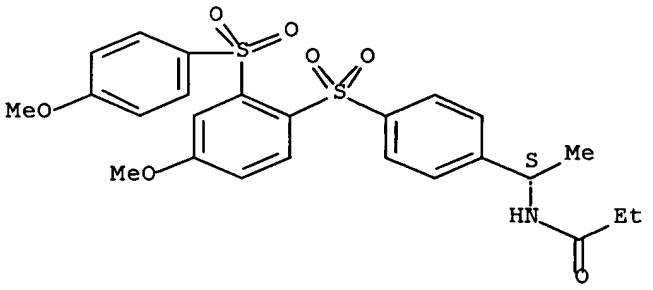
RN 447459-51-0 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



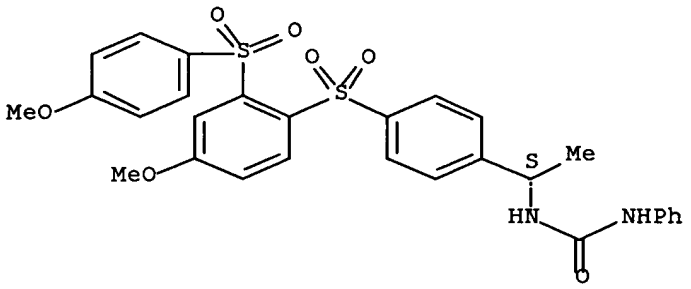
RN 447459-52-1 HCAPLUS
CN Propanamide, N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



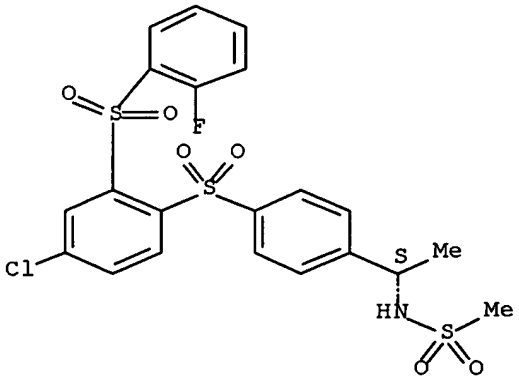
RN 447459-53-2 HCAPLUS
CN Urea, N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



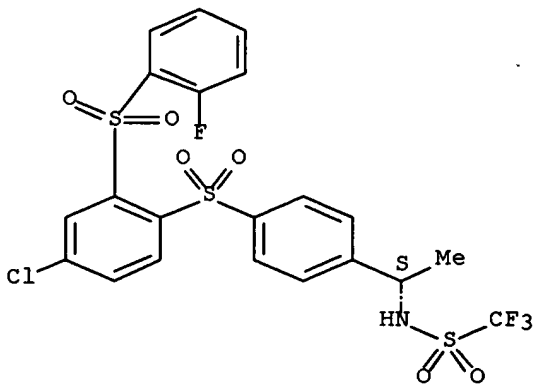
RN 447459-54-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



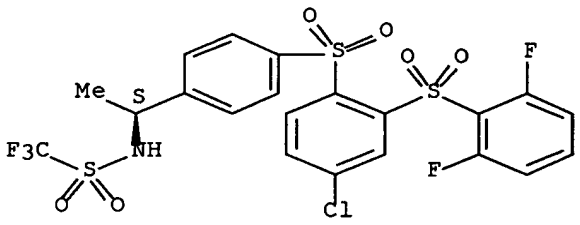
RN 447459-55-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



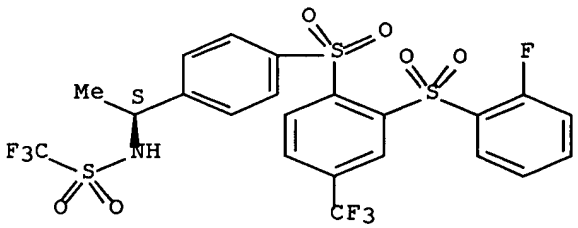
RN 447459-56-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

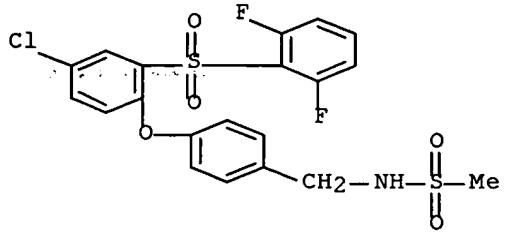


RN 447459-57-6 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

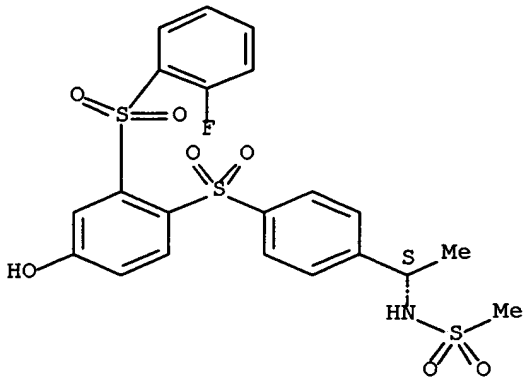


RN 447459-58-7 HCAPLUS
CN Methanesulfonamide, N-[[4-[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)



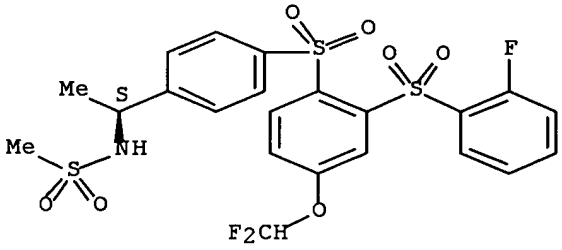
RN 447459-59-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-hydroxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



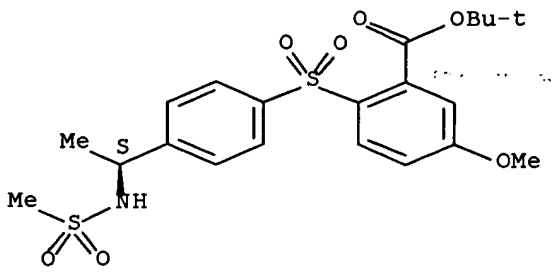
RN 447459-60-1 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-(difluoromethoxy)-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



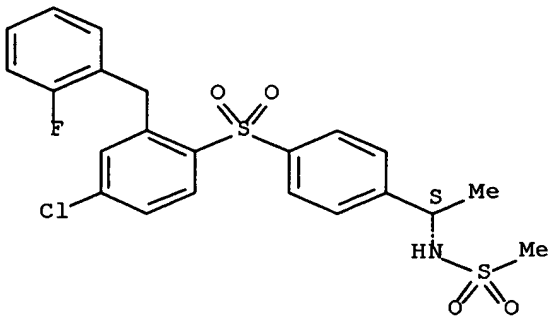
RN 447459-62-3 HCAPLUS
CN Benzoic acid, 5-methoxy-2-[[4-[(1S)-1-[(methylsulfonyl)amino]ethyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



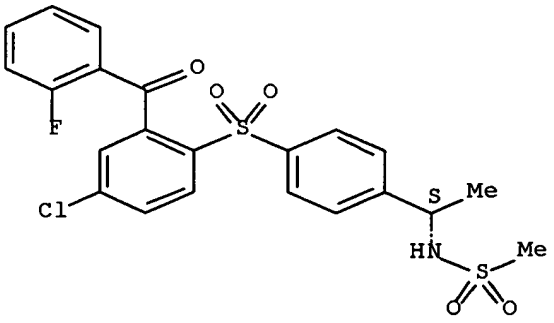
RN 447459-63-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)methyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



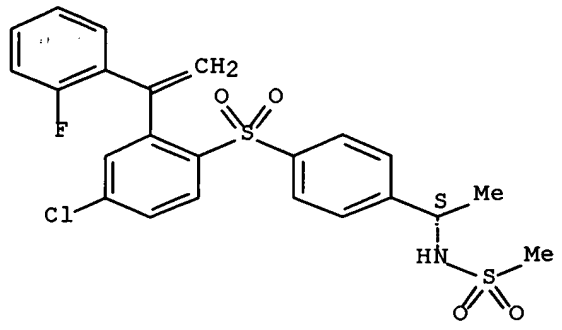
RN 447459-64-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(2-fluorobenzoyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



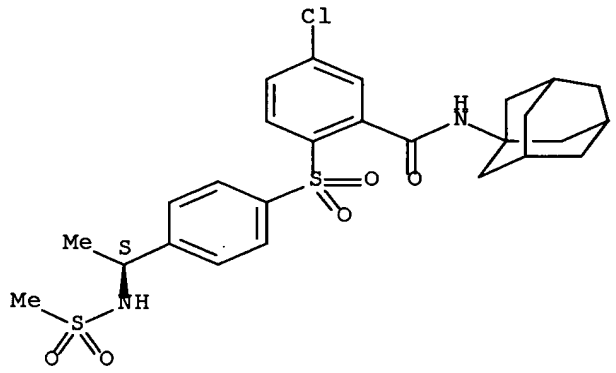
RN 447459-65-6 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[1-(2-fluorophenyl)ethenyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



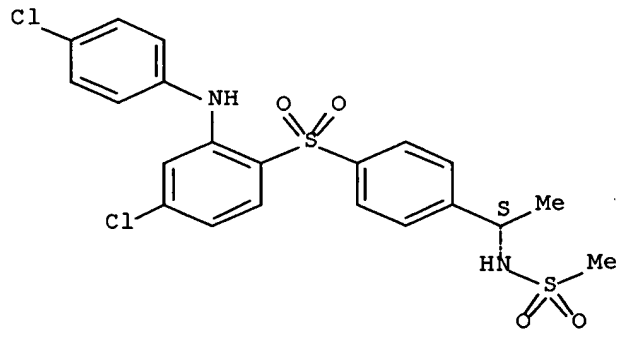
RN 447459-66-7 HCAPLUS
CN Benzamide, 5-chloro-2-[[4-[(1S)-1-[(methylsulfonyl)amino]ethyl]phenyl]sulfonyl]-N-tricyclo[3.3.1.13,7]dec-1-yl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 447459-67-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(4-chlorophenyl)amino]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

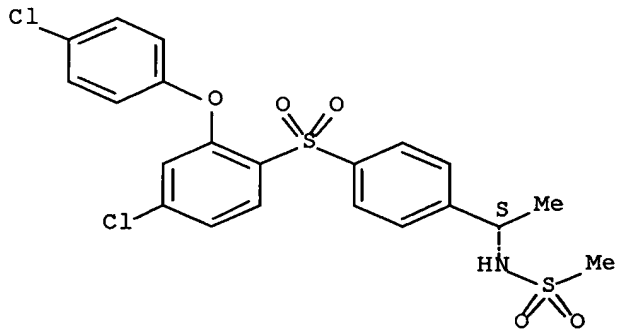
Absolute stereochemistry.



RN 447459-68-9 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(4-chlorophenoxy)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

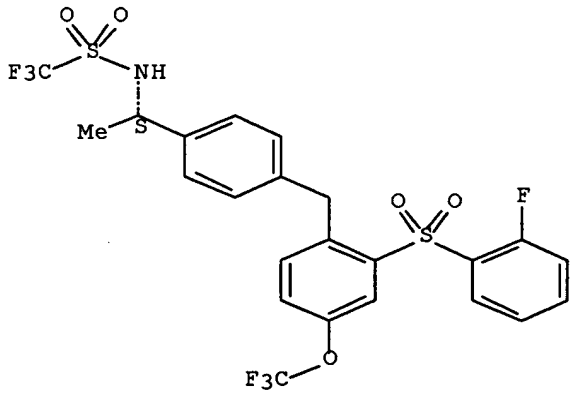
Absolute stereochemistry.



RN 447459-69-0 HCAPLUS

CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

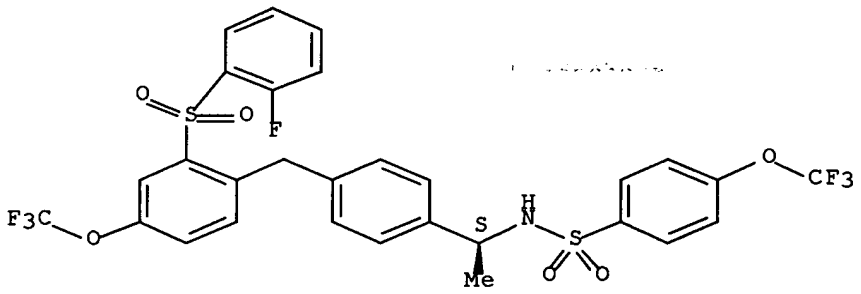
Absolute stereochemistry.



RN 447459-70-3 HCAPLUS

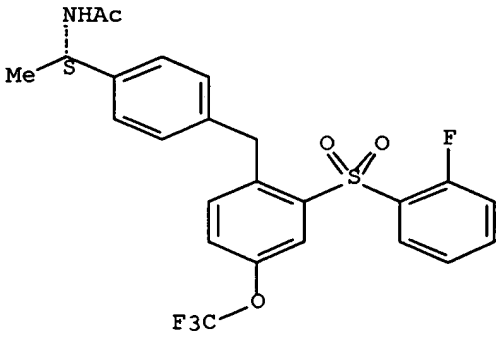
CN Benzenesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



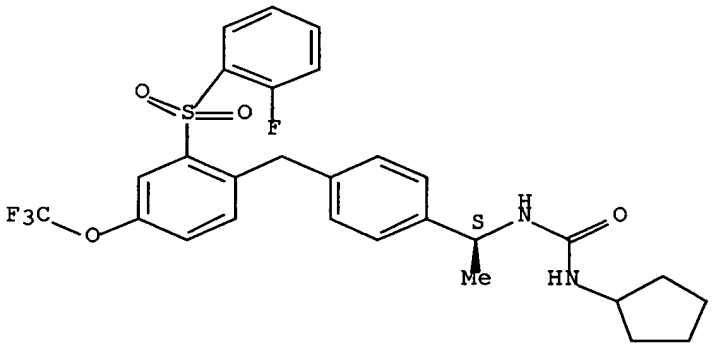
RN 447459-71-4 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



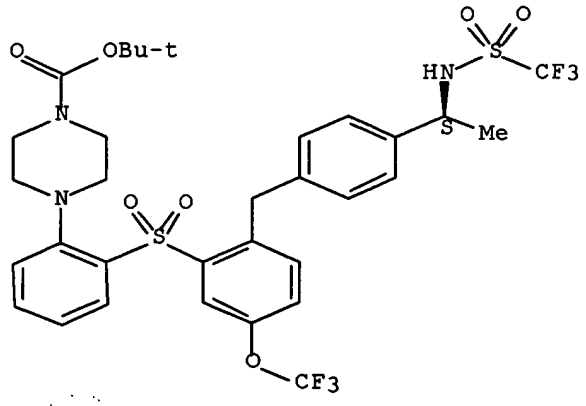
RN 447459-72-5 HCAPLUS
CN Urea, N-cyclopentyl-N'-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



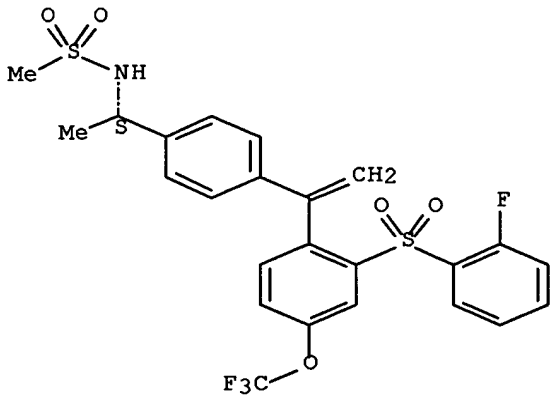
RN 447459-73-6 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[[5-(trifluoromethoxy)-2-[[4-[(1S)-1-[[(trifluoromethyl)sulfonyl]amino]ethyl]phenyl]methyl]phenyl]sulfonyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



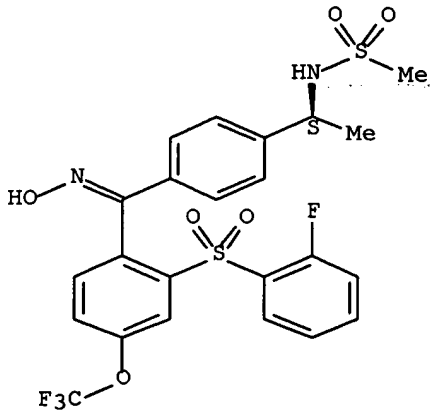
RN 447459-74-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[1-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]ethenyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



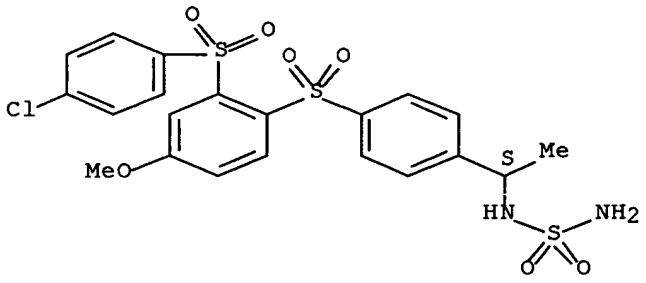
RN 447459-75-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl](hydroxyimino)methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

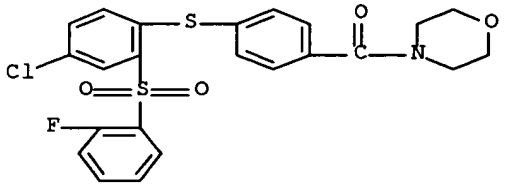


RN 447459-76-9 HCAPLUS
CN Sulfamide, [(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

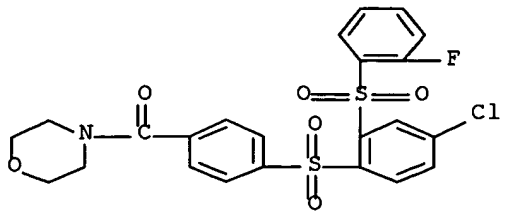
Absolute stereochemistry.



RN 447459-77-0 HCAPLUS
CN Morpholine, 4-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]thio]benzoyl]- (9CI) (CA INDEX NAME)

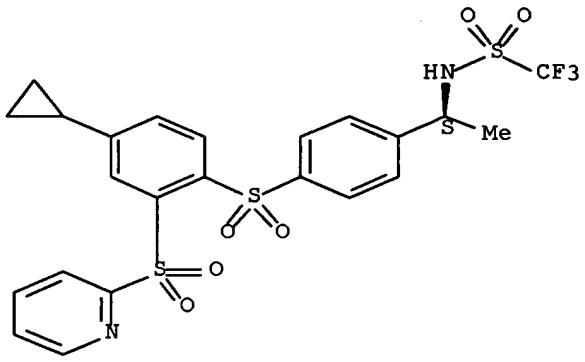


RN 447459-78-1 HCAPLUS
CN Morpholine, 4-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]benzoyl]- (9CI) (CA INDEX NAME)



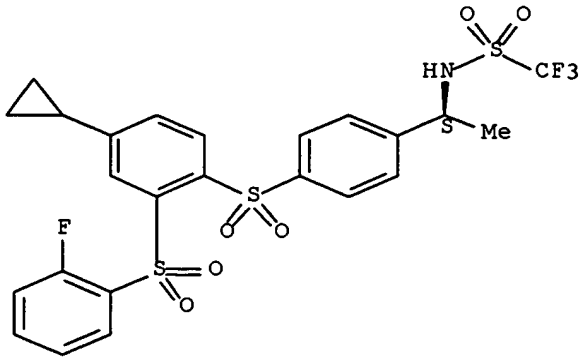
RN 447459-79-2 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 447459-80-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

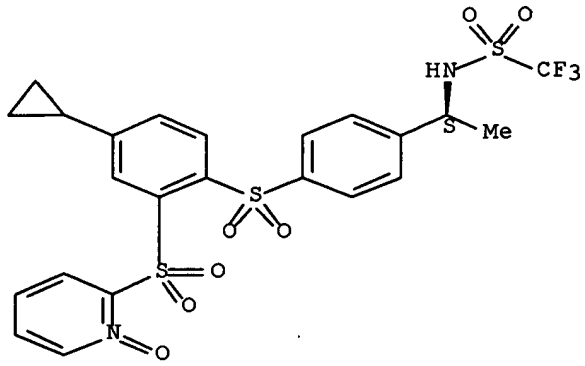
Absolute stereochemistry.



RN 447459-81-6 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-[(1-oxido-2-pyridinyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI)

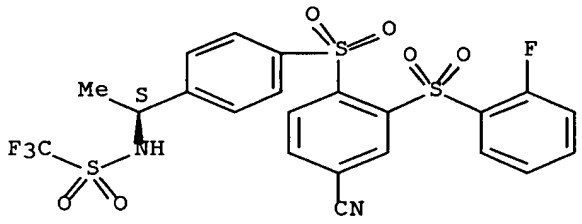
(CA INDEX NAME)

Absolute stereochemistry.



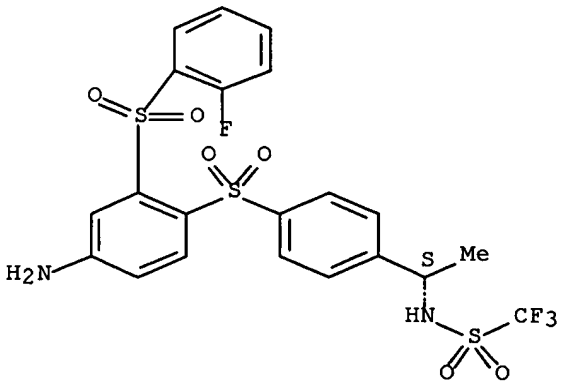
RN 447459-82-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyano-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



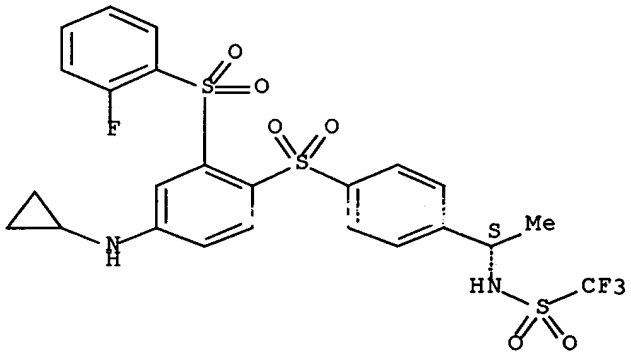
RN 447459-83-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-amino-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



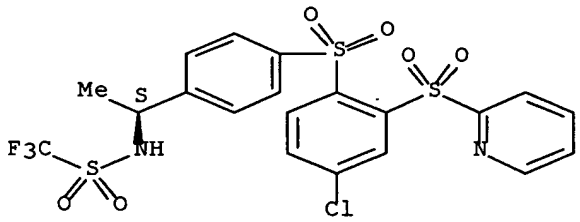
RN 447459-84-9 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-(cyclopropylamino)-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



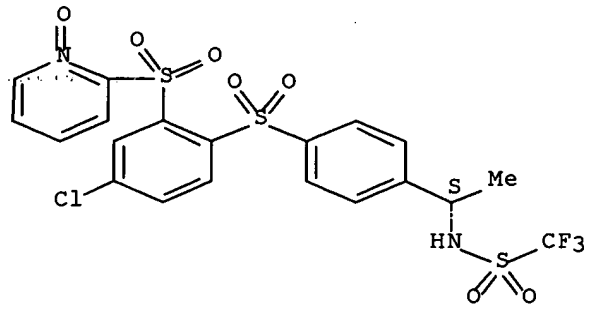
RN 447459-85-0 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



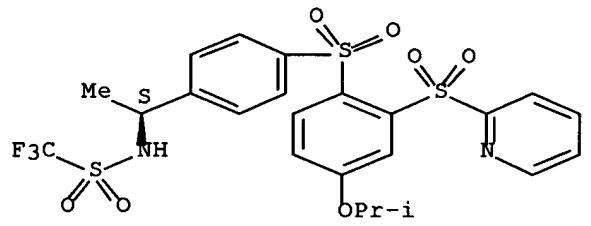
RN 447459-86-1 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(1-oxido-2-pyridinyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



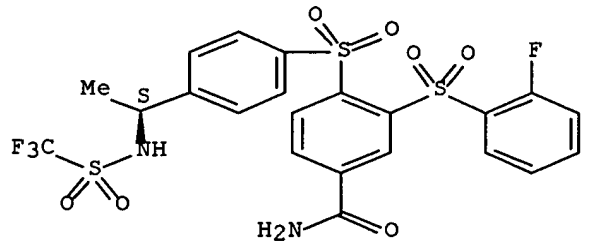
RN 447459-87-2 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[4-(1-methylethoxy)-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



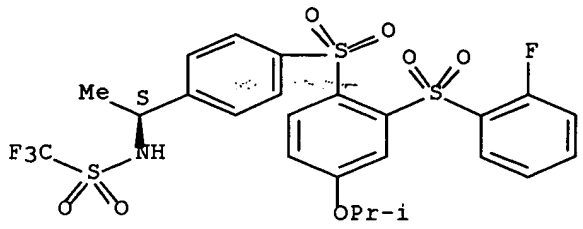
RN 447459-88-3 HCAPLUS
CN Benzamide, 3-[(2-fluorophenyl)sulfonyl]-4-[[4-[(1S)-1-[[(trifluoromethyl)sulfonyl]amino]ethyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



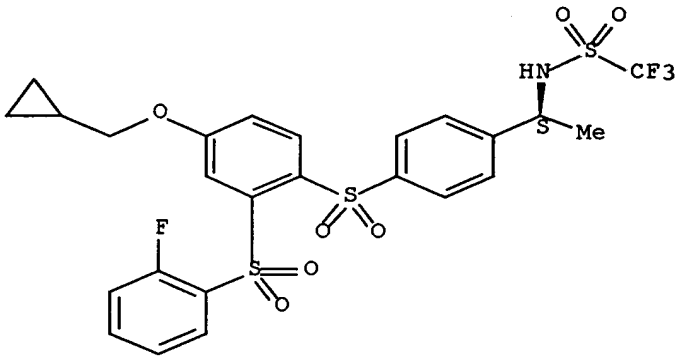
RN 447459-89-4 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(1-methylethoxy)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



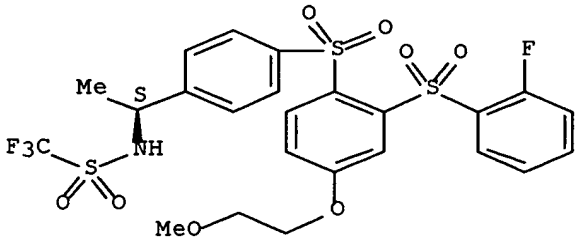
RN 447459-90-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-(cyclopropylmethoxy)-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



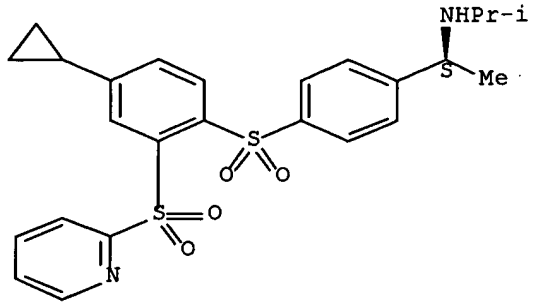
RN 447459-91-8 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(2-methoxyethoxy)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

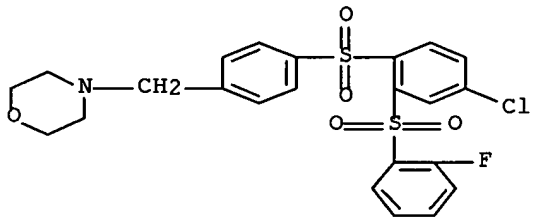


RN 447459-92-9 HCAPLUS
CN Benzenemethanamine, 4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-α-methyl-N-(1-methylethyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

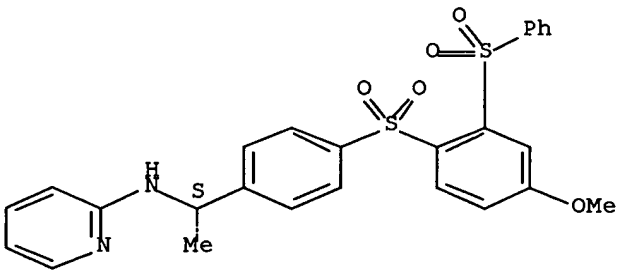


RN 447459-93-0 HCAPLUS
CN Morpholine, 4-[[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



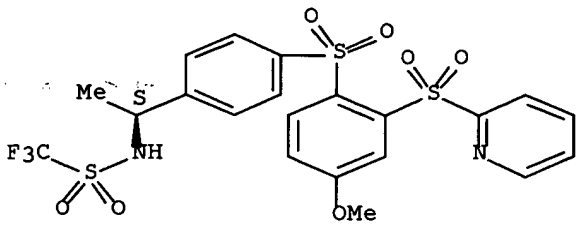
RN 447459-94-1 HCAPLUS
CN 2-Pyridinamine, N-[(1S)-1-[4-[[4-methoxy-2-(phenylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



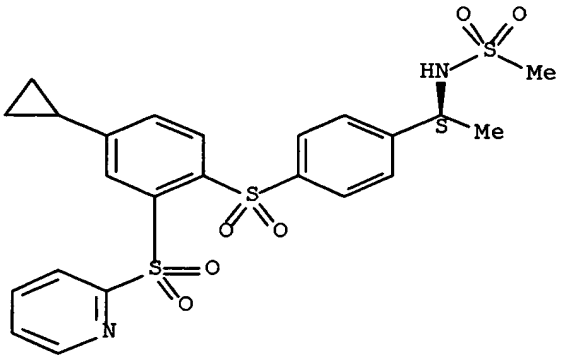
RN 447459-95-2 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[4-methoxy-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

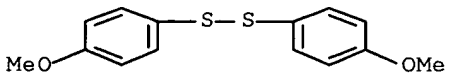


RN 447459-96-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

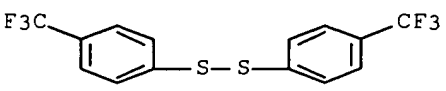
Absolute stereochemistry.



IT 5335-87-5, Bis(4-methoxyphenyl)disulfide 18715-45-2, Bis(4-trifluoromethylphenyl)disulfide 447460-46-0 447460-48-2 447460-49-3 447460-50-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of methylbenzylsulfonamides as cannabinoid receptor ligands)
RN 5335-87-5 HCAPLUS
CN Disulfide, bis(4-methoxyphenyl) (9CI) (CA INDEX NAME)

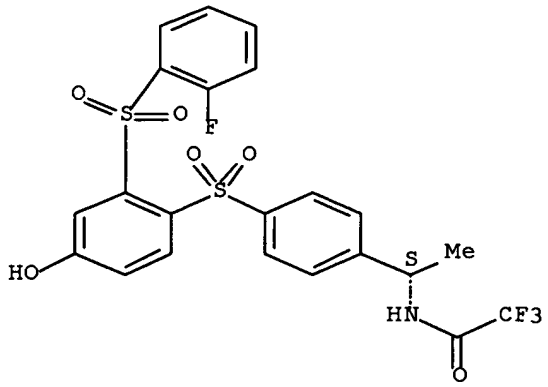


RN 18715-45-2 HCAPLUS
CN Disulfide, bis[4-(trifluoromethyl)phenyl] (9CI) (CA INDEX NAME)



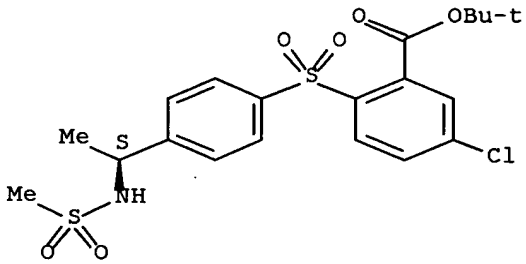
RN 447460-46-0 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-hydroxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



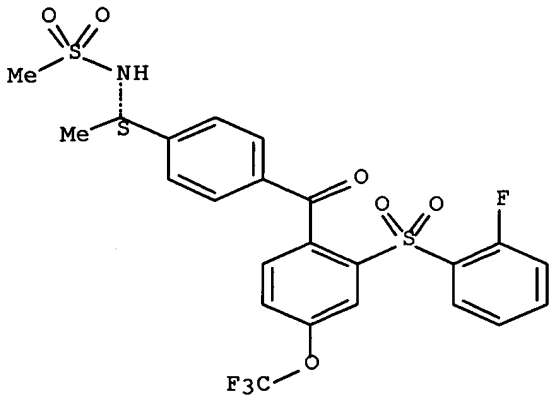
RN 447460-48-2 HCAPLUS
CN Benzoic acid, 5-chloro-2-[[4-[(1S)-1-[(methylsulfonyl)amino]ethyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



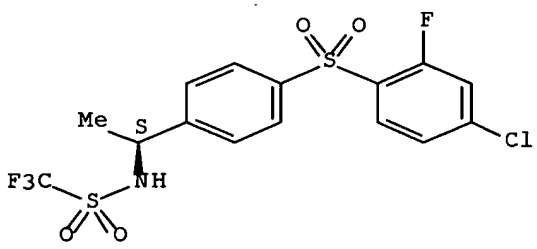
RN 447460-49-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 447460-50-6 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[(4-chloro-2-fluorophenyl)sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 447459-97-4P 447459-98-5P 447459-99-6P
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447460-06-2P 447460-07-3P 447460-08-4P
447460-09-5P 447460-10-8P 447460-11-9P
447460-12-0P 447460-13-1P 447460-14-2P
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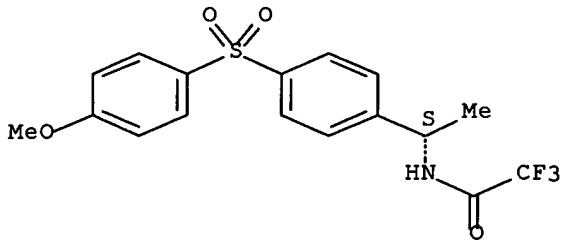
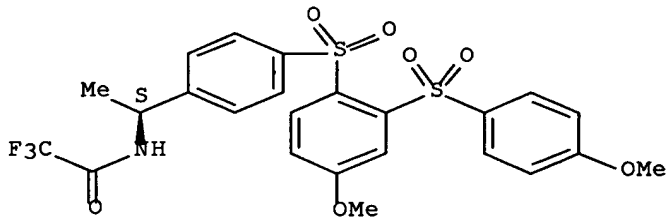
447460-47-1P 447460-51-7P 447460-52-8P
447460-53-9P 447460-54-0P 447460-69-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of methylbenzylsulfonamides as cannabinoid receptor ligands)
RN 447459-97-4 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[(4-methoxyphenyl)sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



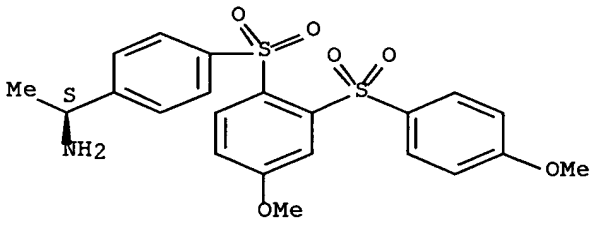
RN 447459-98-5 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



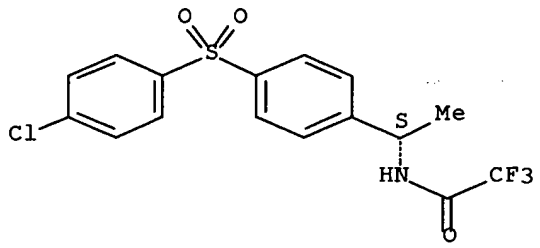
RN 447459-99-6 HCAPLUS
CN Benzenemethanamine, 4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



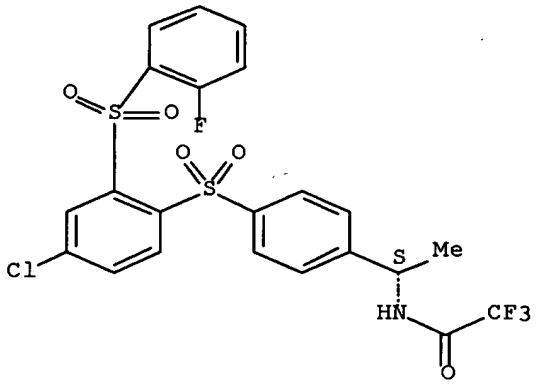
RN 447460-00-6 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chlorophenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



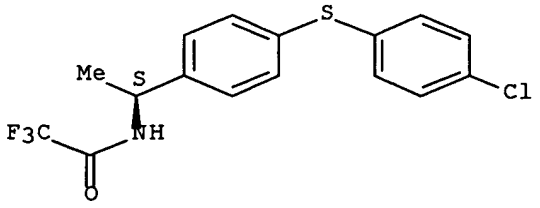
RN 447460-01-7 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



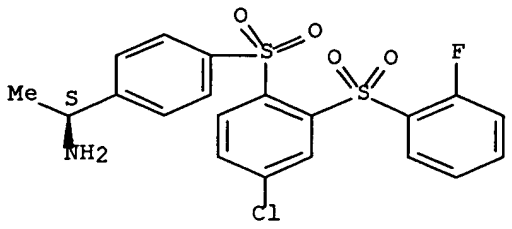
RN 447460-02-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chlorophenyl)thio]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



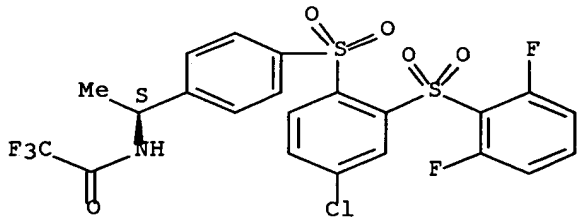
RN 447460-03-9 HCAPLUS
CN Benzenemethanamine, 4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



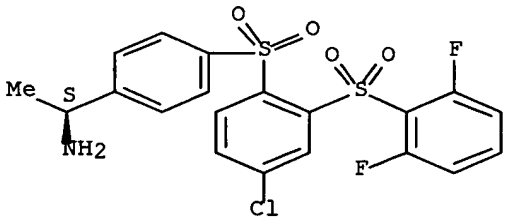
RN 447460-04-0 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

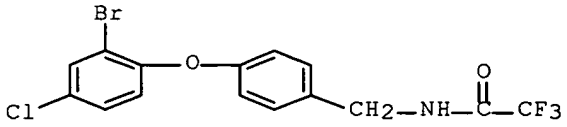


RN 447460-05-1 HCAPLUS
CN Benzenemethanamine, 4-[[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

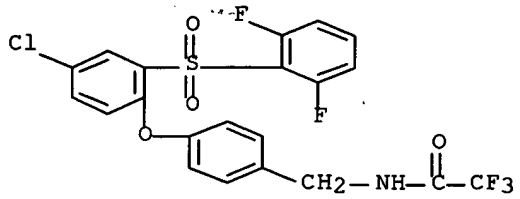
Absolute stereochemistry.



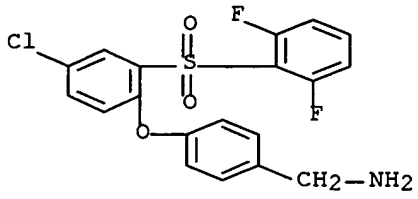
RN 447460-06-2 HCAPLUS
CN Acetamide, N-[[4-(2-bromo-4-chlorophenoxy)phenyl]methyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)



RN 447460-07-3 HCAPLUS
CN Acetamide, N-[[4-[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenoxy]phenyl]methyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

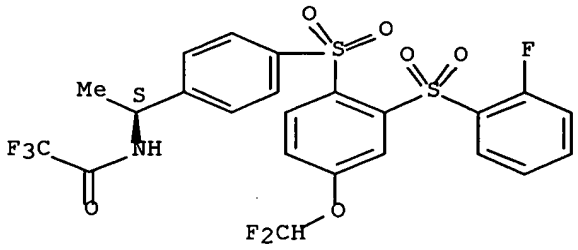


RN 447460-08-4 HCAPLUS
CN Benzenemethanamine, 4-[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenoxy]- (9CI) (CA INDEX NAME)



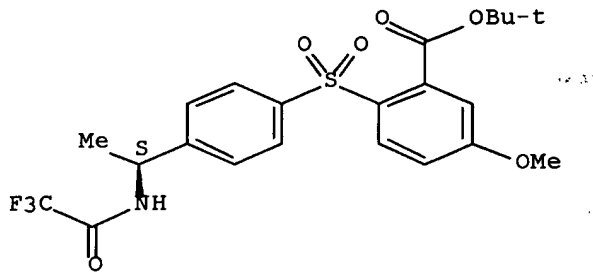
RN 447460-09-5 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-(difluoromethoxy)-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



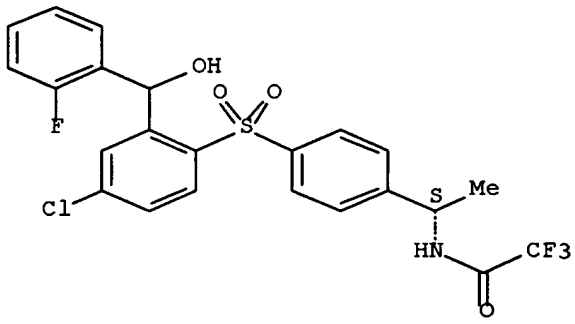
RN 447460-10-8 HCAPLUS
CN Benzoic acid, 5-methoxy-2-[[4-[(1S)-1-[(trifluoroacetyl)amino]ethyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



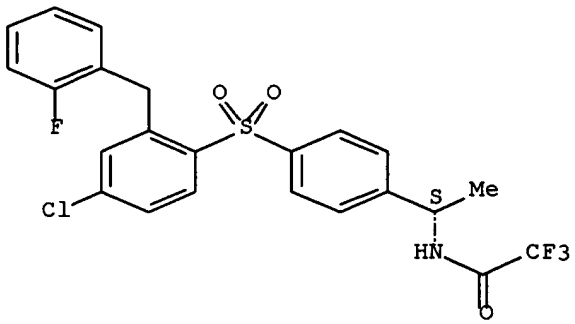
RN 447460-11-9 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)hydroxymethyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



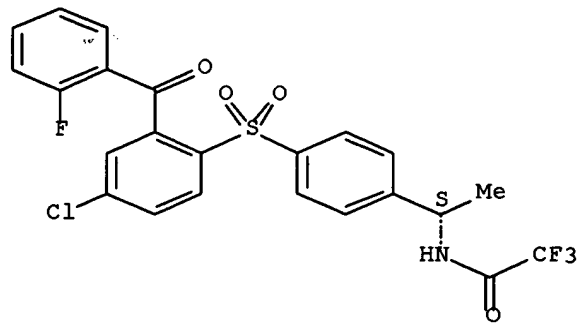
RN 447460-12-0 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)methyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



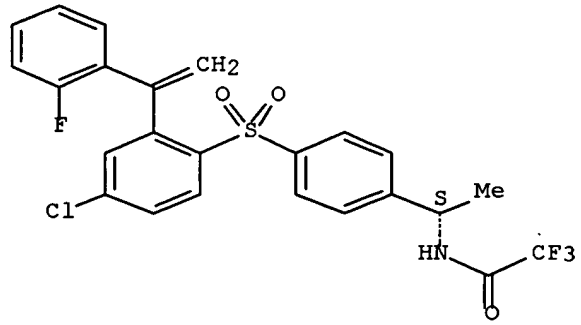
RN 447460-13-1 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-(2-fluorobenzoyl)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



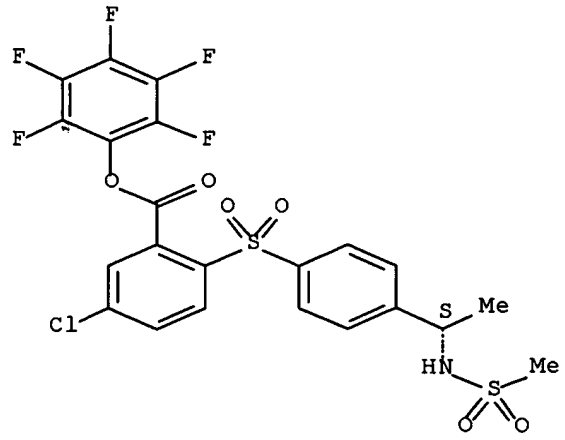
RN 447460-14-2 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[1-(2-fluorophenyl)ethenyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



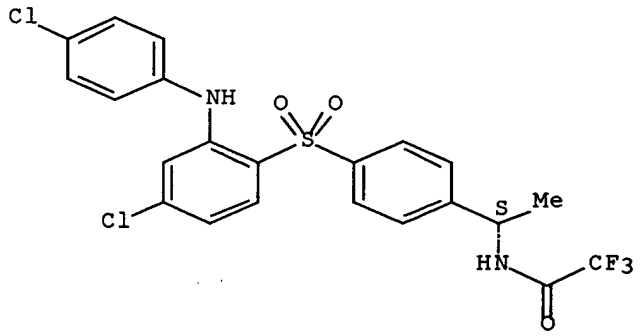
RN 447460-15-3 HCAPLUS
CN Benzoic acid, 5-chloro-2-[[4-[(1S)-1-[(methylsulfonyl)amino]ethyl]phenyl]sulfonyl]-, pentafluorophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



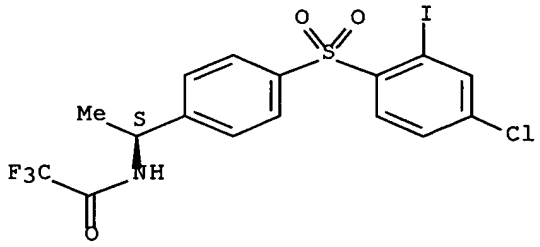
RN 447460-16-4 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(4-chlorophenyl)amino]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



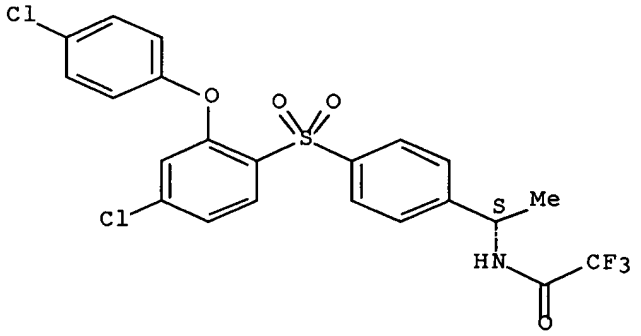
RN 447460-17-5 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chloro-2-iodophenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

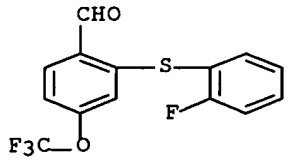


RN 447460-18-6 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-(4-chlorophenoxy)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

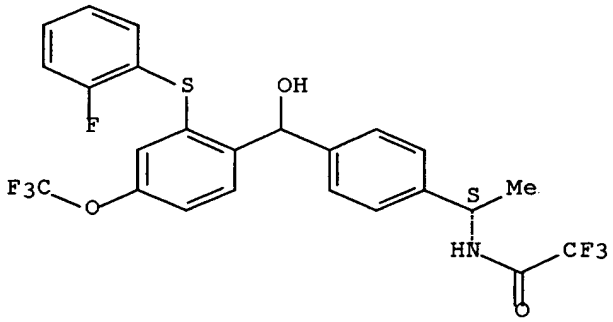


RN 447460-19-7 HCAPLUS
CN Benzaldehyde, 2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



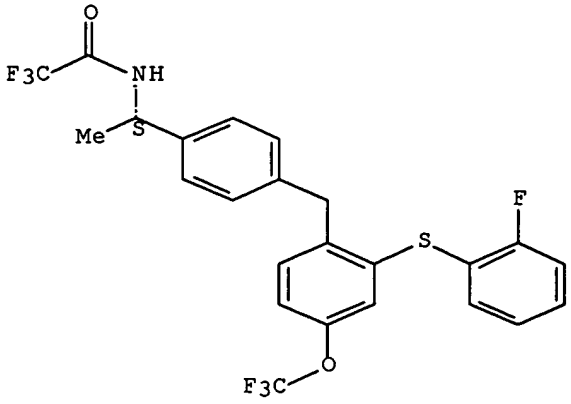
RN 447460-20-0 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)phenyl]hydroxymethyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



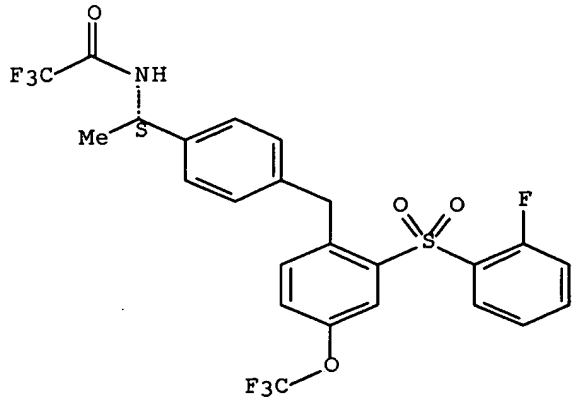
RN 447460-21-1 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



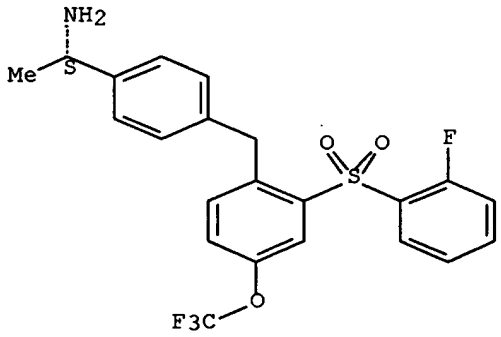
RN 447460-22-2 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



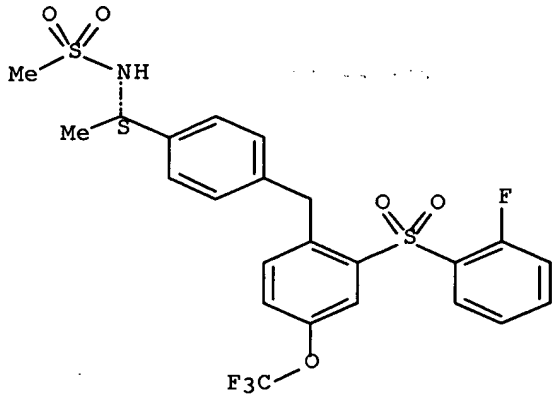
RN 447460-23-3 HCAPLUS
CN Benzenemethanamine, 4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



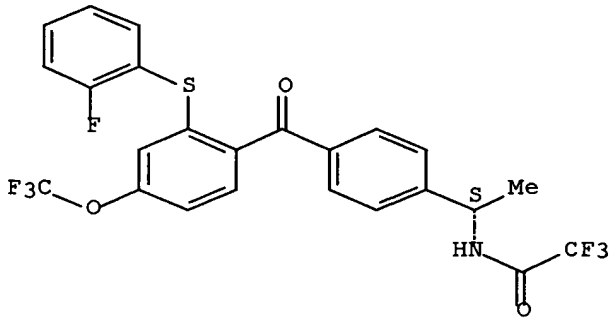
RN 447460-24-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



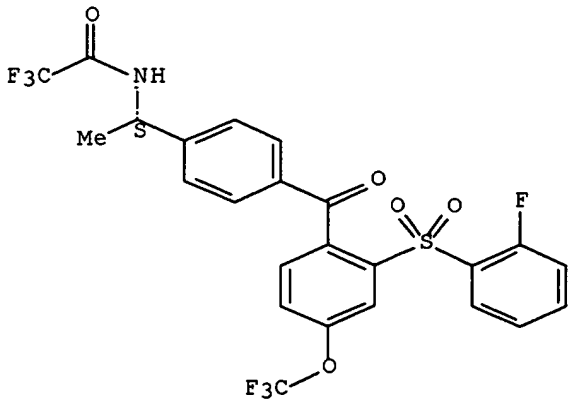
RN 447460-25-5 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



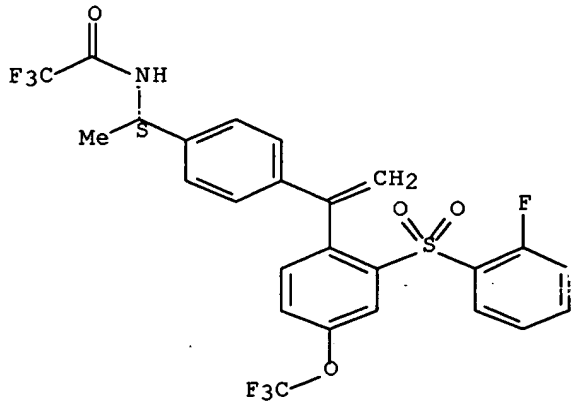
RN 447460-26-6 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



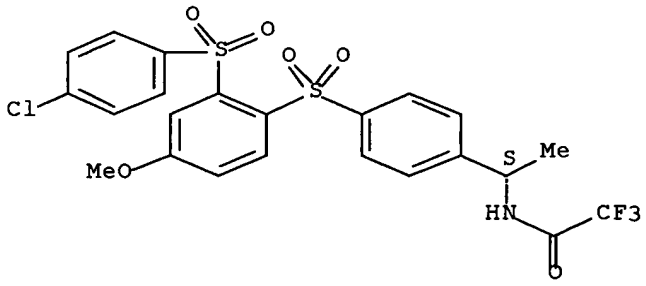
RN 447460-27-7 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[1-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]ethenyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



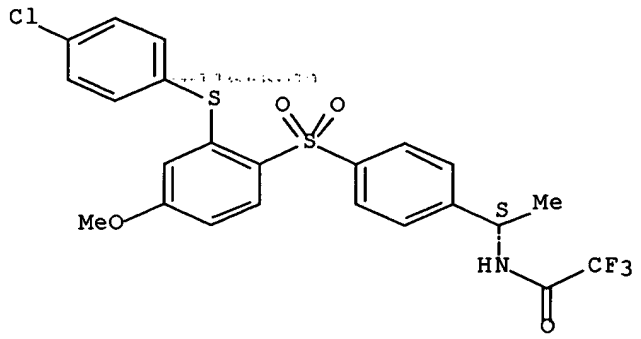
RN 447460-28-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



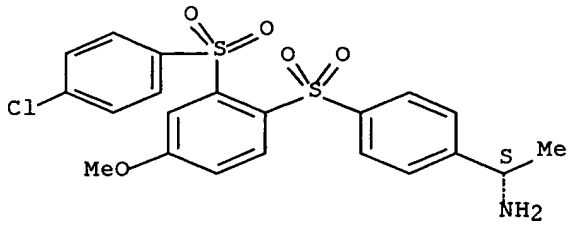
RN 447460-29-9 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)thio]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

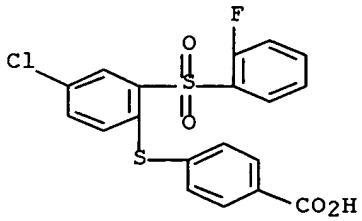


RN 447460-30-2 HCAPLUS
CN Benzenemethanamine, 4-[[2-[(4-chlorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

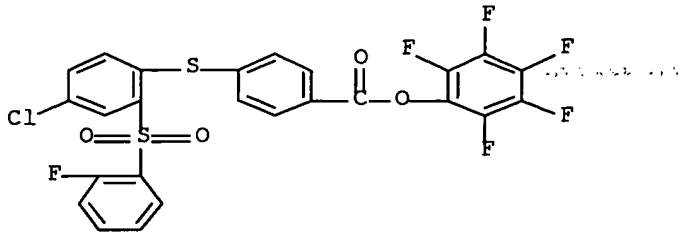
Absolute stereochemistry.



RN 447460-32-4 HCAPLUS
CN Benzoic acid, 4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]thio]- (9CI) (CA INDEX NAME)

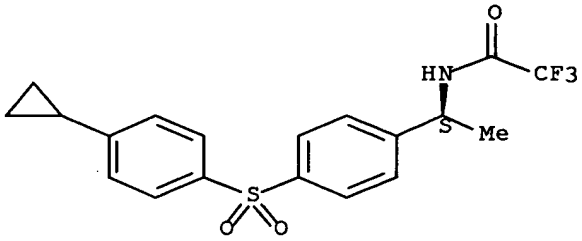


RN 447460-33-5 HCAPLUS
CN Benzoic acid, 4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]thio]-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



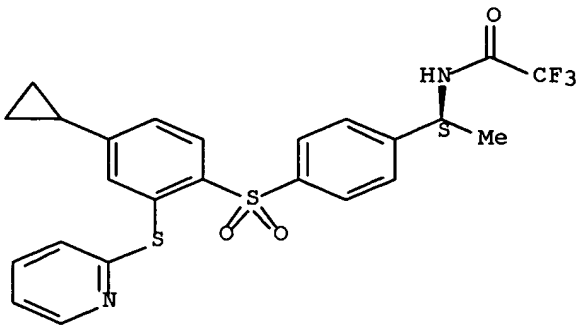
RN 447460-35-7 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-cyclopropylphenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



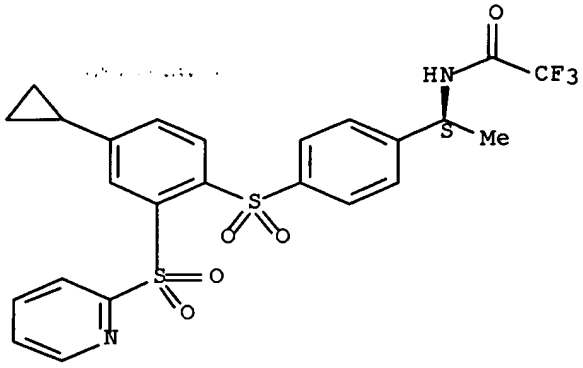
RN 447460-36-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-(2-pyridinylthio)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



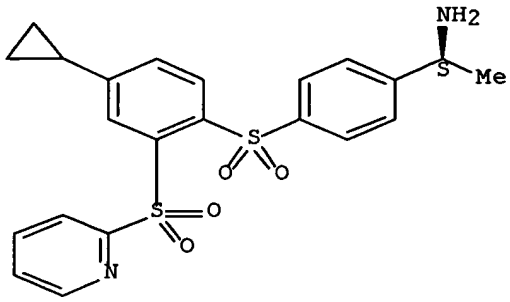
RN 447460-37-9 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



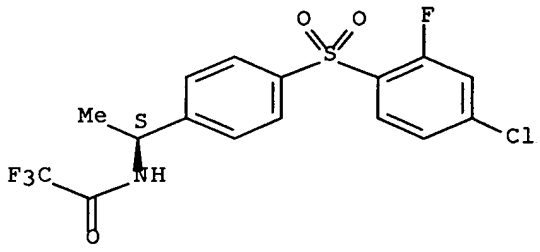
RN 447460-38-0 HCAPLUS
CN Benzenemethanamine, 4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



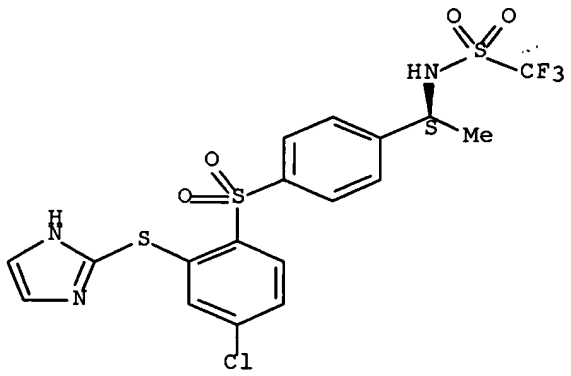
RN 447460-40-4 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chloro-2-fluorophenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



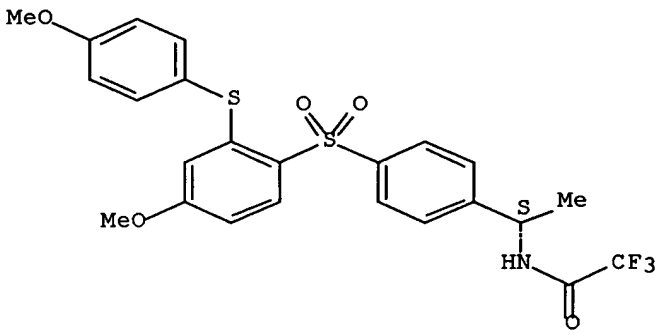
RN 447460-41-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(1H-imidazol-2-ylthio)phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



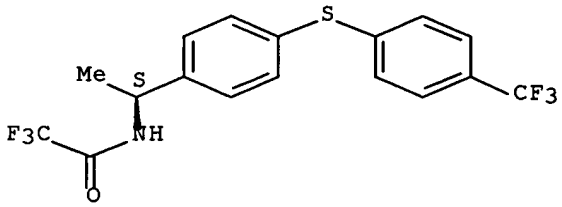
RN 447460-42-6 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)thio]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



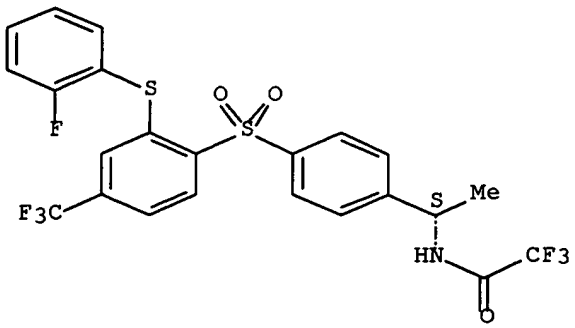
RN 447460-44-8 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[4-(trifluoromethyl)phenyl]thio]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



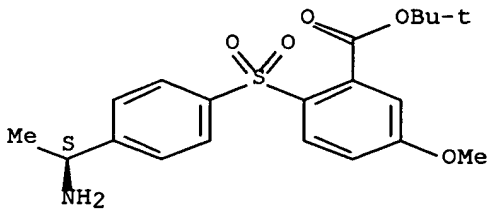
RN 447460-45-9 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)thio]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



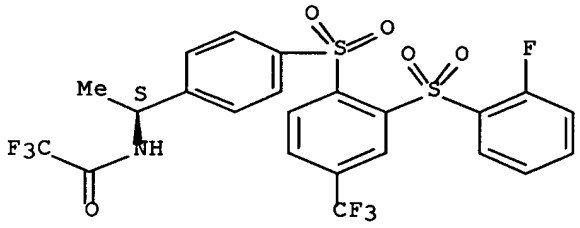
RN 447460-47-1 HCAPLUS
CN Benzoic acid, 2-[[4-[(1S)-1-aminoethyl]phenyl]sulfonyl]-5-methoxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



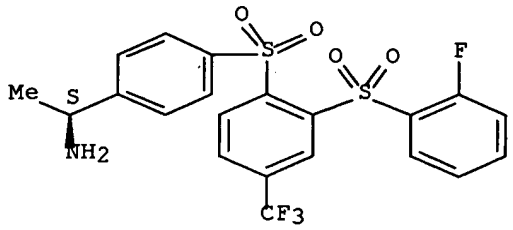
RN 447460-51-7 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

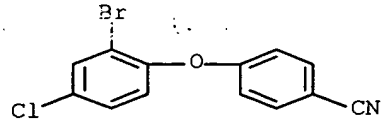


RN 447460-52-8 HCAPLUS
CN Benzenemethanamine, 4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

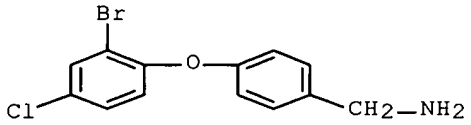
Absolute stereochemistry.



RN 447460-53-9 HCAPLUS
CN Benzonitrile, 4-(2-bromo-4-chlorophenoxy)- (9CI) (CA INDEX NAME)

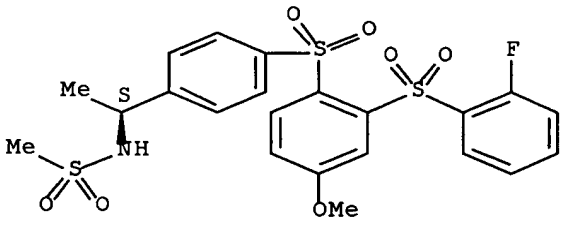


RN 447460-54-0 HCAPLUS
CN Benzenemethanamine, 4-(2-bromo-4-chlorophenoxy)- (9CI) (CA INDEX NAME)



RN 447460-69-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 25 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:950452 HCAPLUS Full-text
DOCUMENT NUMBER: 140:13029
TITLE: Conjugates of an autocrine motility factor receptor ligand and a cytotoxic molecule for use in cancer

therapy
INVENTOR(S): Nabi, Ivan R.
PATENT ASSIGNEE(S): Can.
SOURCE: U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S. Ser. No. 700,844, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003223978	A1	20031204	US 2003-366319	20030214
CA 2238257	AA	19991122	CA 1998-2238257	19980522
WO 9961060	A1	19991202	WO 1999-CA438	19990513

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

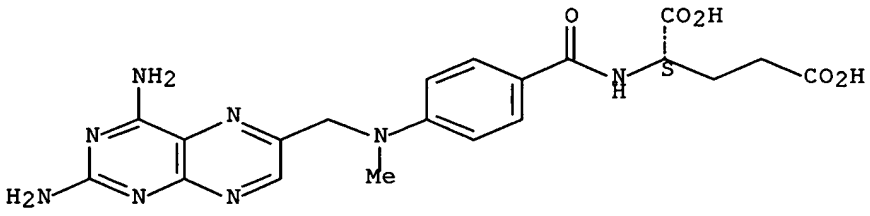
CA 1998-2238257	A	19980522
WO 1999-CA438	W	19990513
US 2001-700844	B2	20010208

AB The invention provides a therapeutic conjugate to specifically kill motile cells, which comprises a first mol. which binds to autocrine motility factor receptor (AMF-R) attached to a second toxic mol. to kill said motile cells, e.g. metastatic tumor cells.

IT 59-05-2D, Methotrexate, conjugates
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(autocrine motility factor receptor ligand conjugate with cytotoxic mol. for cancer therapy)

RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 26 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:777515 HCAPLUS Full-text
DOCUMENT NUMBER: 139:286801
TITLE: Derivatives of isoflavones and their conjugates as estrogen receptor ligands

INVENTOR(S): Kohen, Fortune; Gayer, Batya; Stern, Naftali; Somjen, Dalia

PATENT ASSIGNEE(S): Yeda Research and Development Co. Ltd., Israel; The Medical Research Fund Near the Tel-Aviv Sourasky Medical Center

SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

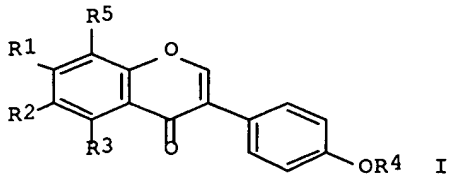
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003079965	A2	20031002	WO 2003-IL224	20030316
WO 2003079965	A3	20040603		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003214609	A1	20031008	AU 2003-214609	20030316
EP 1484966	A2	20041215	EP 2003-710189	20030316
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005096381	A1	20050505	US 2004-943943	20040920
PRIORITY APPLN. INFO.:			IL 2002-148825 A	20020321
			WO 2003-IL224 W	20030316

OTHER SOURCE(S): MARPAT 139:286801

GI



I

AB Isoflavones I [R1 = OH, OMe, OGlc, (un)substituted carboxymethoxy (Q); R2 = H, Q; R3 = H, OH, Q, (un)substituted carboxymethyl (Q1); R4 = H, Me, Q1; R5 = H, Q1] are active as selective estrogen receptor modulators, useful for the treatment of estrogen-related conditions. Conjugates of I, conjugated through one or more of R1-R4, are useful for affinity targeting of drugs, imaging and detection agents to cells having estrogen receptors, particularly estrogen receptors subtype β. Thus, a conjugate of 6-carboxymethylgenistein and dunomycin was prepared and has affinity for several tumor cell lines.

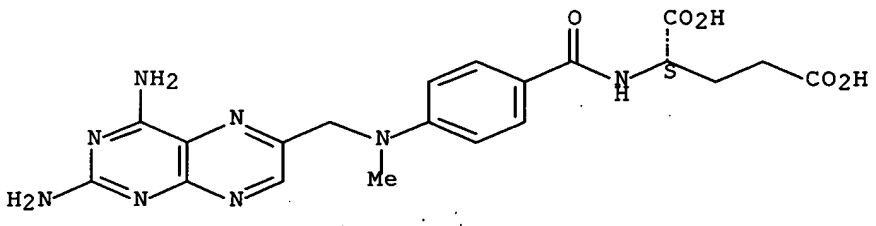
IT 59-05-2D, Methotrexate, isoflavone conjugates

RL: PAC (Pharmacological activity); BIOL (Biological study)
(derivs. of isoflavones and their conjugates as estrogen receptor ligands)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 27 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:575662 HCAPLUS Full-text
DOCUMENT NUMBER: 139:302423
TITLE: Expression and molecular pharmacology of the mouse CRTH2 receptor
AUTHOR(S): Hata, Aaron N.; Zent, Roy; Breyer, Matthew D.; Breyer, Richard M.
CORPORATE SOURCE: Department of Pharmacology, Vanderbilt University School of Medicine, Nashville, TN, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2003), 306(2), 463-470
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

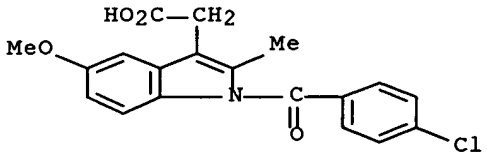
AB Prostaglandin D2 (PGD2), the predominant prostanoid produced by activated mast cells, is implicated in a variety of allergic diseases. PGD2 exerts its effects through two G-protein coupled receptors, DP and CRTH2. PGD2 mediates chemotaxis of eosinophils, basophils, and Th2 cells via CRTH2-evoked signaling, suggesting a role for this receptor in allergic disease. To characterize the mouse CRTH2 ortholog (mCRTH2), we amplified the mCRTH2 receptor gene and expressed it in HEK293 cells. Saturation ligand binding isotherms demonstrated high-affinity binding of [3H]PGD2, with a Kd of 8.8±0.8 nM. Competition binding assays with a panel unlabeled prostanoids demonstrated an order of affinity of 13,14-dihydro-15-keto- PGD2 (DK-PGD2) ≥ 15-deoxy-Δ12,14-PGJ2 (15d-PGJ2) ≥ PGD2 ≥ PGJ2. [3H]PGD2 binding was also displaced by the nonsteroidal anti-inflammatory drug indomethacin, with a Ki value of 1.04±0.13 μM. No [3H]PGD2 displacement was detected using fluribrofen, ibuprofen, or aspirin as competitors at concns. of up to 30 μM. PGD2, DK-PGD2, 15d-PGJ2, and indomethacin each inhibited intracellular cAMP generation in stable transfectant ER293/mCRTH2 cells through a pertussis toxin (PTX) sensitive pathway, consistent with mCRTH2 coupling to a Gi heterotrimeric G-protein. Activation of mCRTH2 elicited chemotaxis of ER293/mCRTH2 cells in response to PGD2, indomethacin, and 15d-PGJ2. MCRTH2-dependent chemotaxis was inhibited by PTX and wortmannin, indicating dependence on Gi and PI 3-kinase signal transduction pathways. These data

provide the first pharmacol. and functional characterization of the mouse CRTH2 receptor.

IT 53-86-1, Indomethacin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(expression of mouse CRTH2 receptor and its ligand binding in relation to cAMP/PI3 kinase signaling and cell migration)

RN 53-86-1 HCAPLUS

CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

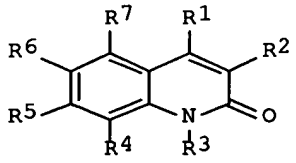
L21 ANSWER 28 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:491224 HCAPLUS Full-text
DOCUMENT NUMBER: 139:69162
TITLE: Preparation of quinolinones as prostaglandin E receptor ligands for treatment of pain, fever, inflammation, and other prostanoid receptor mediated disorders
INVENTOR(S): Dube, Daniel; Deschenes, Denis; Fortin, Rejean; Girard, Yves
PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051878	A1	20030626	WO 2002-CA1914	20021211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2469048	AA	20030626	CA 2002-2469048	20021211
AU 2002350315	A1	20030630	AU 2002-350315	20021211
EP 1458718	A1	20040922	EP 2002-784961	20021211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005520797	T2	20050714	JP 2003-552762	20021211
US 2005222194	A1	20051006	US 2004-498084	20040610

PRIORITY APPLN. INFO.: US 2001-340439P P 20011214
WO 2002-CA1914 W 20021211

OTHER SOURCE(S): MARPAT 139:69162

GI



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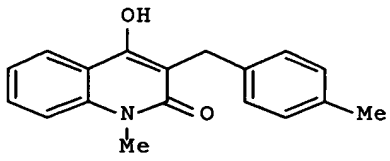


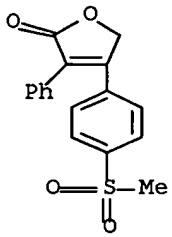
II

AB Title compds. I [wherein R1 = H, halo, OH, N(R8)2, or (un)substituted alkyl, alkenyl, alkoxy, alkylthio, alkanoyl(oxy), alkoxycarbonyl, aryl, aralkyl, aryloxy, aralkoxy, arylthio, aroyl, or aroyloxy; R2 = (un)substituted benzyl, alkyl, alkenyl, or aroyl; R3 = (un)substituted alkyl, alkenyl, alkynyl, aryl, or aralkyl; R4-R7 = independently H, halo, or (un)substituted alkyl; or R3 and R4 may be joined together with the atoms to which they are attached to form a monocyclic ring; R8 = H or (un)substituted alkyl, alkenyl, or alkanoyl; and pharmaceutically acceptable salts, hydrates, esters, or tautomers thereof] were prepared as prostaglandin E receptor ligands (no data). For example, reaction of N-methyl-4-hydroxy-2-quinolone with 4-methylbenzaldehyde in the presence of Et3SiH and TFA in toluene gave II. I and pharmaceutical compns. comprising I may be useful for the treatment of pain, fever, inflammation, and a broad variety of prostagladin E mediated diseases and conditions (no data).

IT 162011-90-7, Rofecoxib 169590-42-5, Celecoxib
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(co-administration agent; preparation of quinolinone prostaglandin E receptor ligands for treatment of pain, fever, inflammation, and other prostanoid mediated diseases)

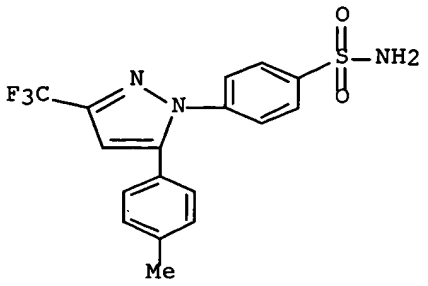
RN 162011-90-7 HCAPLUS

CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 169590-42-5 HCAPLUS

CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

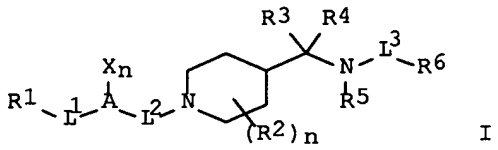
L21 ANSWER 29 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:396851 HCAPLUS Full-text
DOCUMENT NUMBER: 138:401607
TITLE: Preparation of piperidino cannabinoid receptor ligands
INVENTOR(S): Friary, Richard J.; Kozlowski, Joseph A.; Shankar, Bandarpalle B.; Wong, Michael K. C.; Zhou, Guowel; Lavey, Brian J.; Shih, Neng-Yang; Tong, Ling; Chen, Lei; Shu, Youheng
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 148 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003042174	A1	20030522	WO 2002-US36185	20021112
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2466440	AA	20030522	CA 2002-2466440	20021112
US 2004010013	A1	20040115	US 2002-292778	20021112
US 7071213	B2	20060704		
EP 1444203	A1	20040811	EP 2002-784433	20021112
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002014164	A	20040928	BR 2002-14164	20021112
CN 1585749	A	20050223	CN 2002-822675	20021112
JP 2005509032	T2	20050407	JP 2003-544011	20021112
NZ 532291	A	20051125	NZ 2002-532291	20021112
ZA 2004003685	A	20050523	ZA 2004-3685	20040513
NO 2004002435	A	20040611	NO 2004-2435	20040611
US 2005282861	A1	20051222	US 2005-197979	20050805
PRIORITY APPLN. INFO.:			US 2001-332911P	P 20011114
			US 2002-292778	A3 20021112

WO 2002-US36185 W 20021112

OTHER SOURCE(S): MARPAT 138:401607

GI



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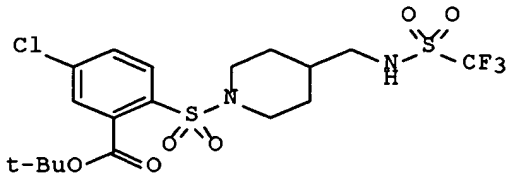


II

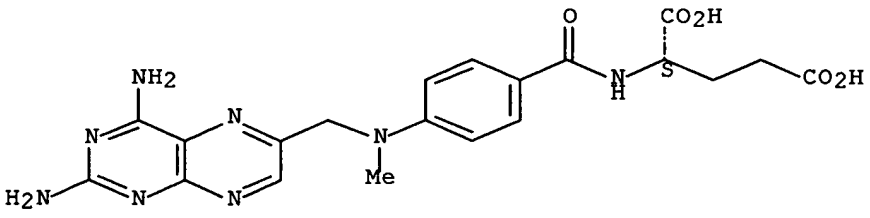
AB Title compds. I [L1 = bond, CH2, CO, CO2, SO2, etc.; L2 = CH2, CH(alkyl), C(alkyl)2, etc.; L3 = bond, CO, SO2; R1 = H, halo, alkyl, haloalkyl, cycloalkyl, etc.; R2 = H, OH, halo, CF3, alkoxy, etc.; R3-4 = H, alkyl, taken together form a carbonyl group; R5 = H, alkyl; R6 = H, alkyl, haloalkyl, cycloalkyl, amino, etc.; n = 0-3] are prepared For instance, 4-(trifluoroacetamidomethyl)piperidine•TFA salt is reacted with p-chlorobenzenesulfonyl chloride (CH2Cl2, Et3N), the resulting sulfonamide functionalized ortho to the sulfonyl group (THF, n-BuLi, Boc2O), the trifluoroacetyl group removed (MeOH, K2CO3) and the amine refunctionalized with trifluoromethanesulfonic anhydride to give II. Compds. of the invention are found to exhibit cannabinoid CB2 receptor binding activity in the range of 0.1 to 1000 nM and possess anti-inflammatory and immunomodulatory activity.

IT 59-05-2, Methotrexate 599-79-1, Sulfasalazine
75706-12-6, Leflunomide 83881-52-1, Zyrtec
153439-40-8, Allegra 162011-90-7, Vioxx
169590-42-5, Celebrex
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combination pharmaceutical; preparation of substituted piperidino cannabinoid receptor ligands for treatment of inflammatory disorders)

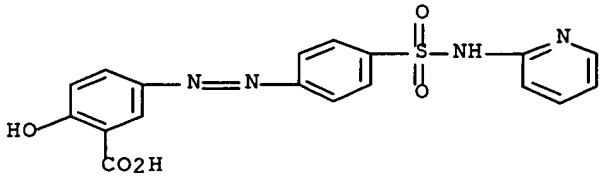
RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

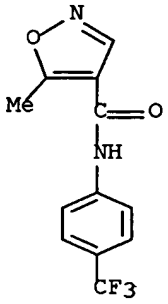
Absolute stereochemistry.



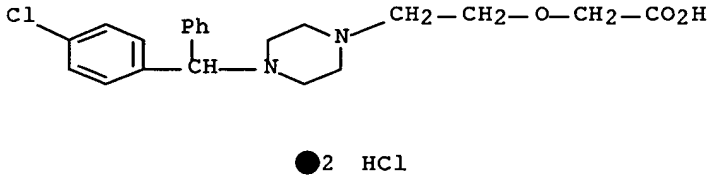
RN 599-79-1 HCAPLUS
CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)



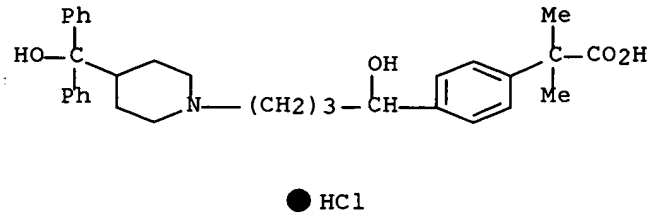
RN 75706-12-6 HCAPLUS
CN 4-Isoxazolecarboxamide, 5-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



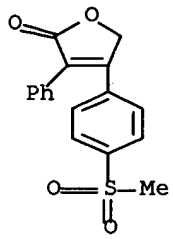
RN 83881-52-1 HCAPLUS
CN Acetic acid, [2-[4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl]ethoxy]-, dihydrochloride (9CI) (CA INDEX NAME)



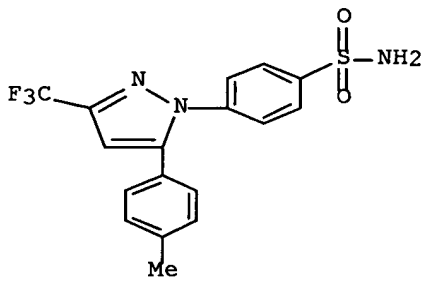
RN 153439-40-8 HCAPLUS
CN Benzeneacetic acid, 4-[1-hydroxy-4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]butyl]-α,α-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



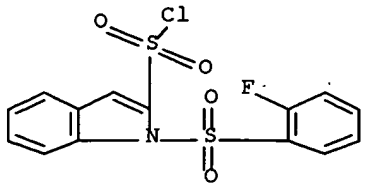
RN 162011-90-7 HCAPLUS
CN 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 169590-42-5 HCAPLUS
CN Benzenesulfonamide, 4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



IT 530116-15-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted piperidino cannabinoid receptor ligands for treatment of inflammatory disorders)
RN 530116-15-5 HCAPLUS
CN 1H-Indole-2-sulfonyl chloride, 1-[(2-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

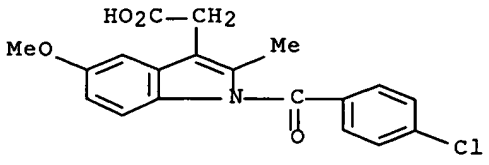


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 30 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:338232 HCAPLUS Full-text
DOCUMENT NUMBER: 140:55887
TITLE: A simple ELISA for screening ligands of peroxisome proliferator-activated receptor γ
AUTHOR(S): Cho, Min Chul; Lee, Hae Sook; Kim, Jae Hwa; Choe, Yong Kyung; Hong, Jin Tae; Paik, Sang Gi; Yoon, Do Young
CORPORATE SOURCE: Laboratory of Cellular Biology, Korea Research Institute of Bioscience and Biotechnology, Daejon, 305-600, S. Korea
SOURCE: Journal of Biochemistry and Molecular Biology (2003), 36(2), 207-213
CODEN: JBMBE5; ISSN: 1225-8687
PUBLISHER: Biochemical Society of the Republic of Korea
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Peroxisome proliferator-activated receptors (PPARs) are orphan nuclear hormone receptors that are known to control the expression of genes that are involved in lipid homeostasis and energy balance. PPARs activate gene transcription in response to a variety of compds., including hypolipidemic drugs. Most of these compds. have high affinity to the ligand-binding domain (LBD) of PPARs and cause a conformational change within PPARs. As a result, the receptor is converted to an activated mode that promotes the recruitment of co-activators such as the steroid receptor co-activator-1 (SRC-1). Based on the activation mechanism of PPARs (the ligand binding to PPARγ induces interactions of the receptor with transcriptional co-activators), we performed Western blot and ELISA. These showed that the indomethacin, a PPARγ ligand, increased the binding between PPARγ and SRC-1 in a ligand dose-dependent manner. These results suggested that the in vitro conformational change of PPARγ by ligands was also induced, and increased the levels of the ligand-dependent interaction with SRC-1. Collectively, we developed a novel and useful ELISA system for the mass screening of PPARγ ligands. This screening system (based on the interaction between PPARγ and SRC-1) may be a promising system in the development of drugs for metabolic disorders.

IT 53-86-1, Indomethacin
RL: ANT (Analyte); ANST (Analytical study)
(ELISA for screening ligands of peroxisome proliferator-activated receptor γ based on its interaction with steroid receptor co-activator-1)
RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 31 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:832916 HCAPLUS Full-text
DOCUMENT NUMBER: 137:347511
TITLE: Steroid and xenobiotic receptor SXR and its use in control of protein gene expression and in gene therapy
INVENTOR(S): Evans, Ronald M.
PATENT ASSIGNEE(S): The Salk Institute for Biological Studies, USA
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

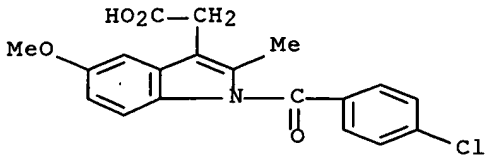
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002086063	A2	20021031	WO 2002-US12161	20020416
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003104519	A1	20030605	US 2001-840008	20010420
US 6911537	B2	20050628		

PRIORITY APPLN. INFO.:		
US 2001-840008	A1	20010420
US 1998-5286	A2	19980109
US 1999-227718	A2	19990108
US 1999-458366	A2	19991209

AB Use of steroid and xenobiotic receptor SXR to control expression of protein genes or therapeutic genes is disclosed. Thus, expression of both human CYP3A4 and rat CYP3A23 genes in rat hepatocytes producing human SXR was stimulated by rifampicin.

IT 53-86-1, Indomethacin
RL: BSU (Biological study, unclassified); BIOL (Biological study) (as ligand for SXR in induction of expression of cytochrome P 450 genes; steroid and xenobiotic-sensing nuclear receptor SXR and its use in xenobiotic inducible expression system)

RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L21 ANSWER 32 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:832624 HCAPLUS Full-text
DOCUMENT NUMBER: 137:333525
TITLE: Estrogen receptor ligands for therapy of multiple sclerosis and other autoimmune diseases
INVENTOR(S): Voskuhl, Rhonda R.
PATENT ASSIGNEE(S): The Regents of the University of California, USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002085374	A1	20021031	WO 2002-US13407		20020425
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
US 2002183299	A1	20021205	US 2002-131834		20020424
US 6936599	B2	20050830			
EP 1397143	A1	20040317	EP 2002-729034		20020425
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
US 2005239762	A1	20051027	US 2005-151040		20050613
PRIORITY APPLN. INFO.:			US 2001-286842P	P	20010425
			US 2002-131834	A	20020424
			WO 2002-US13407	W	20020425

AB The present invention discloses administering steroid hormones to mammals to treat autoimmune related diseases, more particularly, Th1-mediated (cell-mediated) autoimmune diseases including: multiple sclerosis (MS), rheumatoid arthritis (RA), autoimmune thyroiditis and uveitis. Most preferably the invention is used to treat a patient with a therapeutically effective amount of estriol of 8 mg once daily via oral administration to treat the symptoms or prevent the onset of multiple sclerosis. A kit for treating a patient having an autoimmune disease comprising: at least at least one primary agent being an estrogen or estrogen receptor active agent at a therapeutically effective dosage in an effective dosage form; and at least one secondary agent in an effective dosage form.

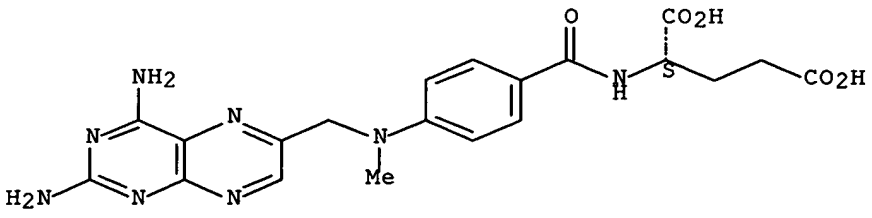
IT 59-05-2, Methotrexate
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(estrogen receptor ligand in combination with other

pharmaceutical agents for treating multiple sclerosis and other autoimmune diseases)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 33 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:615563 HCAPLUS Full-text

DOCUMENT NUMBER: 137:169310

TITLE: Preparation of α-methylbenzylsulfonamides as cannabinoid receptor ligands

INVENTOR(S): Kozlowski, Joseph A.; Shih, Neng-Yang; Lavey, Brian J.; Rizvi, Razia K.; Shankar, Bandarpalle B.; Spitler, James M.; Tong, Ling; Wolin, Ronald; Wong, Michael K.

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 134 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

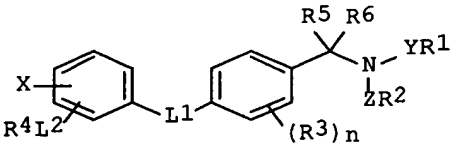
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002062750	A1	20020815	WO 2002-US3672	20020207
WO 2002062750	C2	20030918		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2436659	AA	20020815	CA 2002-2436659	20020207
EP 1368308	A1	20031210	EP 2002-740074	20020207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002006955	A	20040309	BR 2002-6955	20020207
JP 2004530649	T2	20041007	JP 2002-562710	20020207
NZ 526782	A	20050527	NZ 2002-526782	20020207
ZA 2003005933	A	20041101	ZA 2003-5933	20030731

NO 2003003505	A	20031007	NO 2003-3505		20030807
PRIORITY APPLN. INFO.:			US 2001-267375P	P	20010208
			US 2001-292600P	P	20010522
			WO 2002-US3672	W	20020207

OTHER SOURCE(S): MARPAT 137:169310
GI



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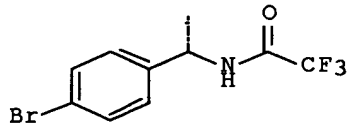
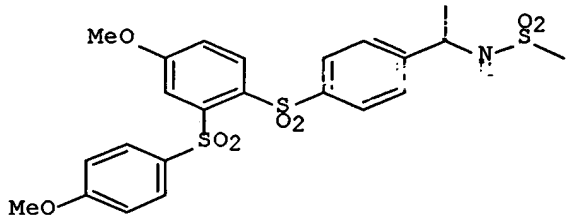


II



III

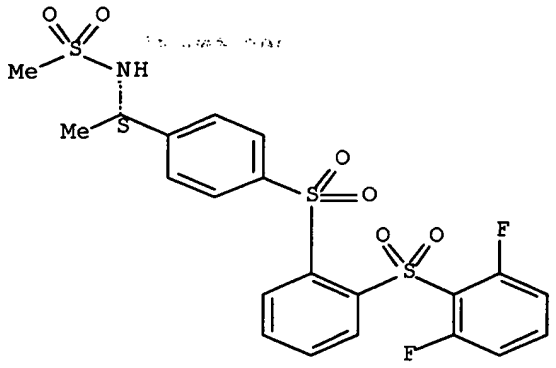
AB Title compds. [I; R1 = H, alkyl, haloalkyl, cycloalkyl, cycloalkylamino, aralkyl, heteroaryl, amino, (substituted) aryl, etc.; R2, R5, R6 = H, alkyl; R3 = H, alkyl, Cl, F, CF3, OCF2H, OCF3, OH, alkoxy; R4 = H, (substituted) alkyl, alkoxy, cycloalkyl, alkenyl, aryl, PhCH2, heteroaryl, arylamino, heteroarylamino, cycloalkylamino, etc.; L1 = alkylene, alkenylene, CO, C(R2)2, CHOR2, NOR5, SO2, SO, S, O, NR2, NR2CO, CHCF3, CF2; L2 = bond, alkylene, CO, C(R2)2, NR2, NR2SO2, CONR2, S, SO, SO2, NOR5, CR2OH, etc.; X = H, halo, CF3, cyano, OCF2H, OCF3, alkyl, cycloalkyl, cycloalkoxy, alkoxy, heteroalkyl, CO2R2, NHR2, arylamino, OSO2R2, etc.; Y, Z = bond, CH2, SO2, CO; R1YNZR2 = atoms to form a heterocycle; n = 0-4], were prepared for treatment of cancer, inflammatory disease, immunomodulatory disease, or respiratory disease (no data). Thus, (S)-α-methylbenzylamine was stirred with (F3CCO)2O in CH2Cl2; the mixture was then treated with MeSO3H and dibromodimethylhydantoin to give 32% intermediate (II). II in THF at -78° was treated with MeLi and then with 4-MeOC6H4SO2Cl followed by warming to room temperature to give 65% di-Ph sulfone derivative The latter in THF at -78° was treated with BuLi then with bis(4-methoxyphenyl)disulfide to give crude disulfide coupling product, which was treated with MCPBA in CH2Cl2 to give 45% bissulfone. This was deprotected with LiOH in H2O/dioxane followed by treatment with MeSO2Cl to give title compound (III).

IT 447459-44-1P 447459-45-2P 447459-46-3P
447459-47-4P 447459-48-5P 447459-49-6P
447459-50-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of methylbenzylsulfonamides as cannabinoid receptor ligands)

RN 447459-44-1 HCAPLUS

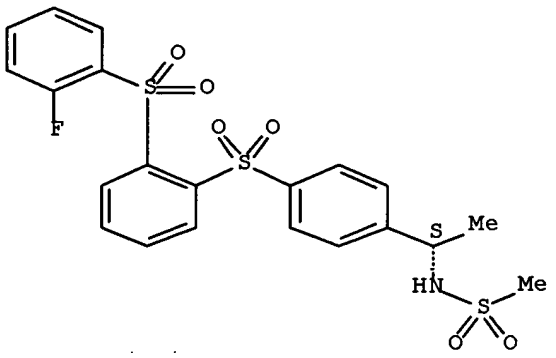
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



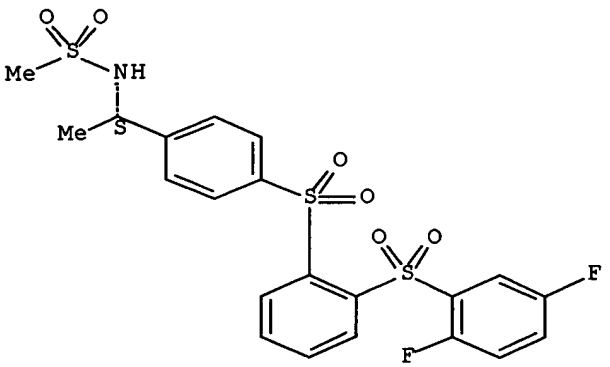
RN 447459-45-2 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



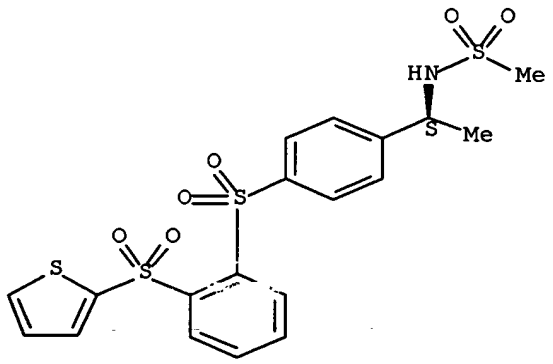
RN 447459-46-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2,5-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



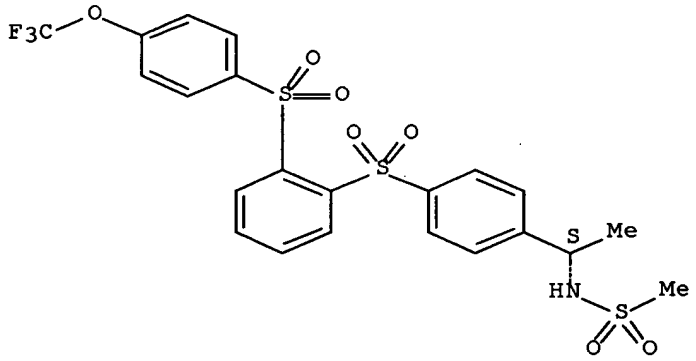
RN 447459-47-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-(2-thienylsulfonyl)phenyl]sulfonyl]ph
enyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



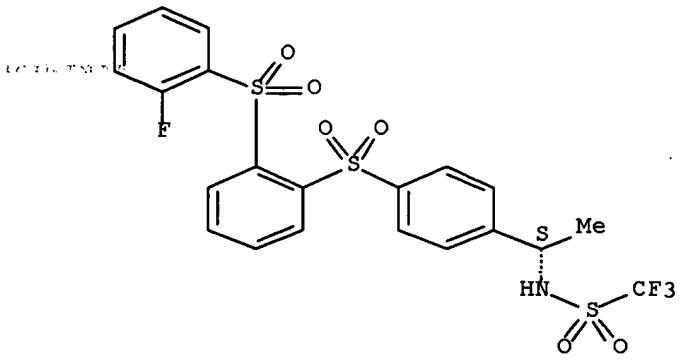
RN 447459-48-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[[4-(trifluoromethoxy)phenyl]sulfonyl
]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



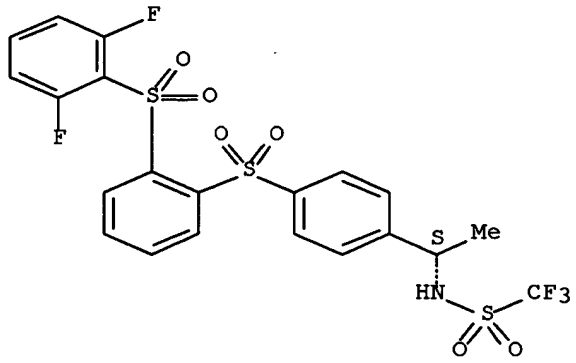
RN 447459-49-6 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-
fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



RN 447459-50-9 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 447459-51-0P 447459-52-1P 447459-53-2P
447459-54-3P 447459-55-4P 447459-56-5P
447459-57-6P 447459-58-7P 447459-59-8P
447459-60-1P 447459-62-3P 447459-63-4P
447459-64-5P 447459-65-6P 447459-66-7P
447459-67-8P 447459-68-9P 447459-69-0P
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447459-73-6P 447459-74-7P 447459-75-8P
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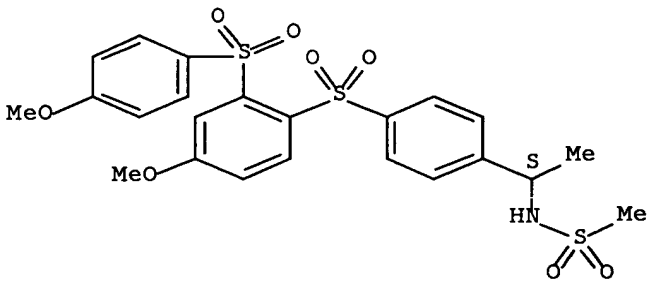
447459-79-2P 447459-80-5P 447459-81-6P
447459-82-7P 447459-83-8P 447459-84-9P
447459-85-0P 447459-86-1P 447459-87-2P
447459-88-3P 447459-89-4P 447459-90-7P
447459-91-8P 447459-92-9P 447459-93-0P
447459-94-1P 447459-95-2P 447459-96-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of methylbenzylsulfonamides as cannabinoid receptor ligands)
RN 447459-51-0 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

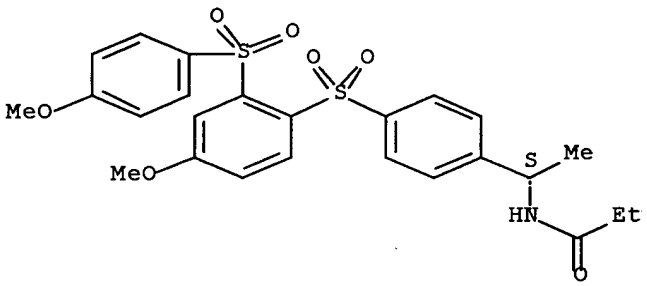
Absolute stereochemistry.



RN 447459-52-1 HCAPLUS

CN Propanamide, N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

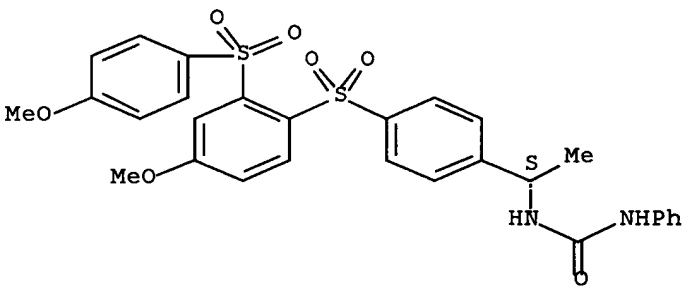
Absolute stereochemistry.



RN 447459-53-2 HCAPLUS

CN Urea, N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)

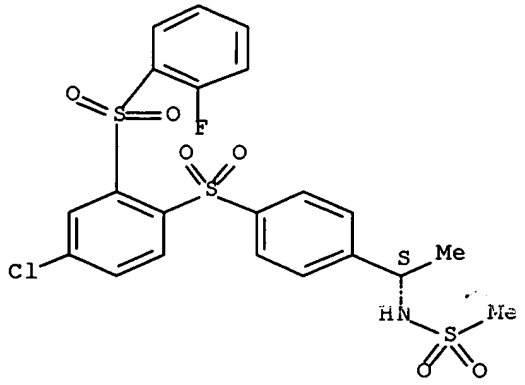
Absolute stereochemistry.



RN 447459-54-3 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

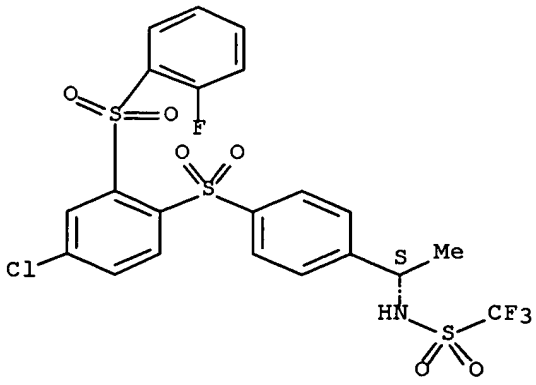
Absolute stereochemistry.



RN 447459-55-4 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

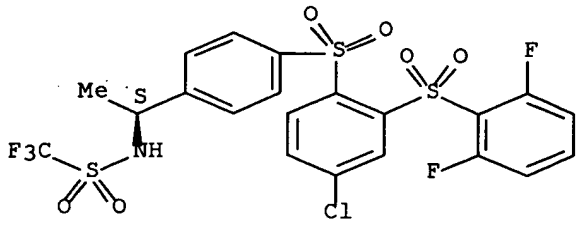
Absolute stereochemistry.



RN 447459-56-5 HCAPLUS

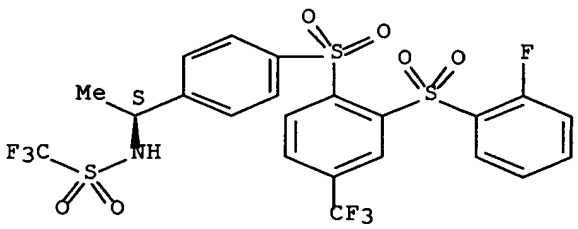
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

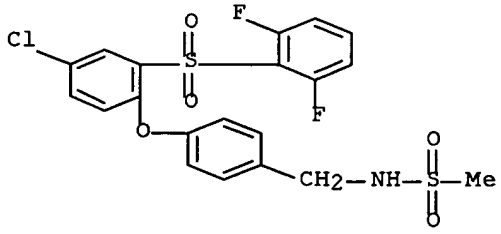


RN 447459-57-6 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

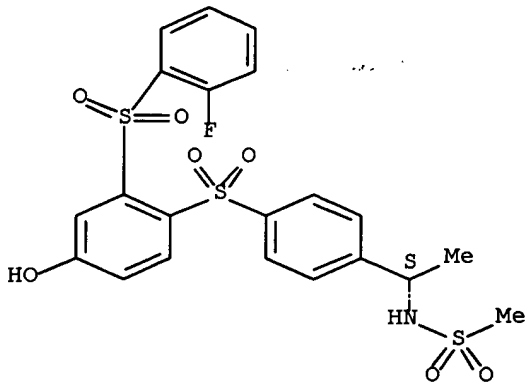


RN 447459-58-7 HCAPLUS
CN Methanesulfonamide, N-[[4-[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)



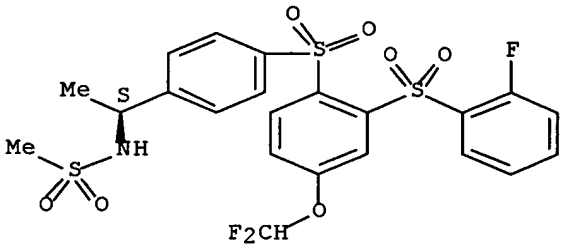
RN 447459-59-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-hydroxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



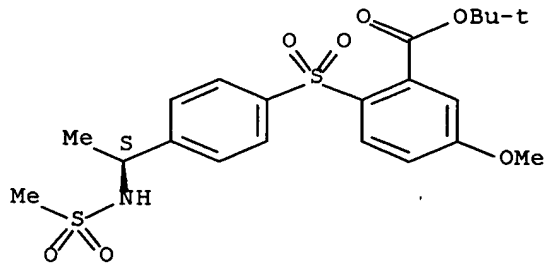
RN 447459-60-1 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-(difluoromethoxy)-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



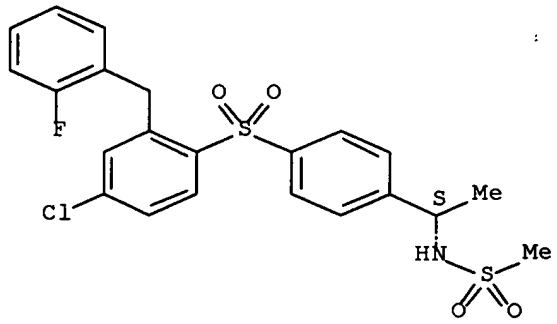
RN 447459-62-3 HCAPLUS
CN Benzoic acid, 5-methoxy-2-[[4-[(1S)-1-[(methylsulfonyl)amino]ethyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



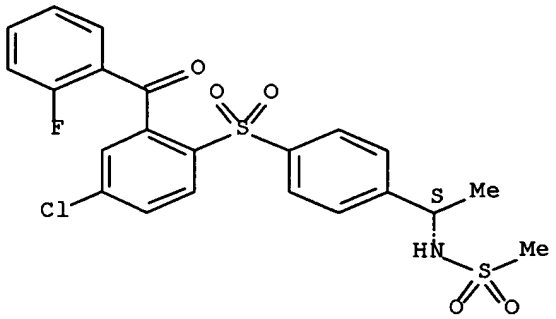
RN 447459-63-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)methyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



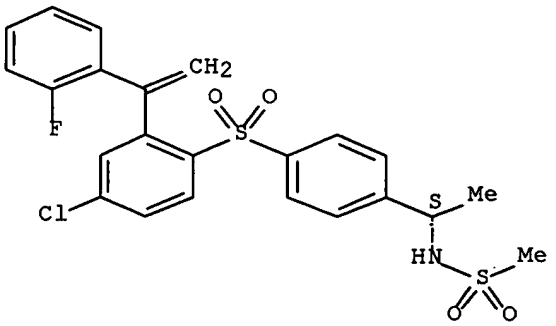
RN 447459-64-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(2-fluorobenzoyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 447459-65-6 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[1-(2-fluorophenyl)ethenyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

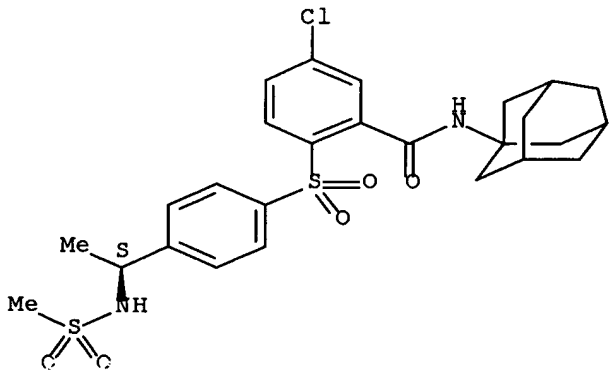
Absolute stereochemistry.



RN 447459-66-7 HCAPLUS
CN Benzamide, 5-chloro-2-[[4-[(1S)-1-[(methylsulfonyl)amino]ethyl]phenyl]sulf

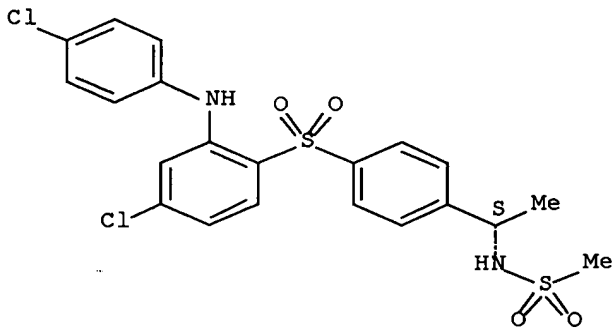
onyl]-N-tricyclo[3.3.1.13,7]dec-1-yl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



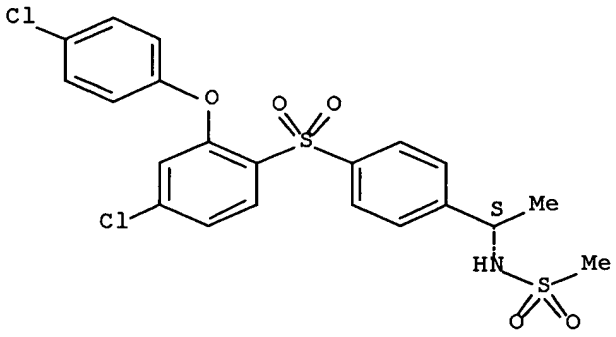
RN 447459-67-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(4-chlorophenyl)amino]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



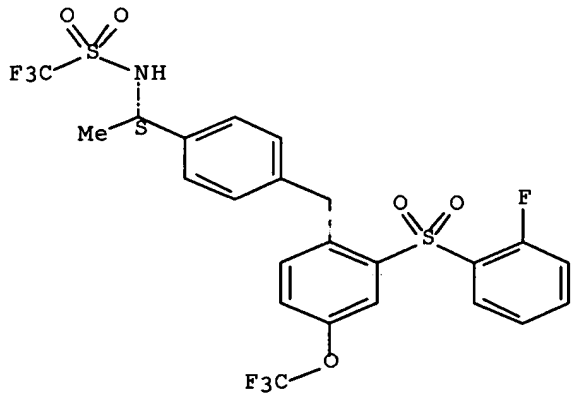
RN 447459-68-9 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(4-chlorophenoxy)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



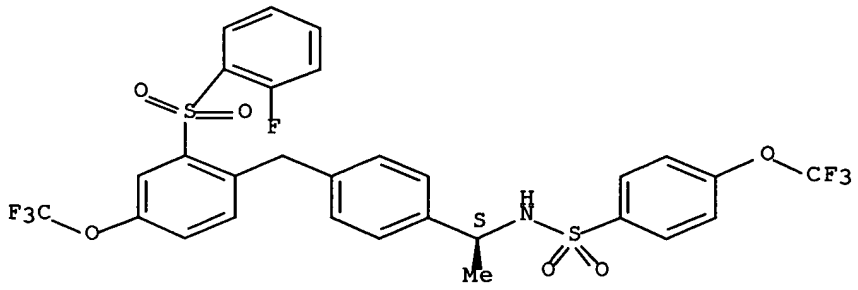
RN 447459-69-0 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



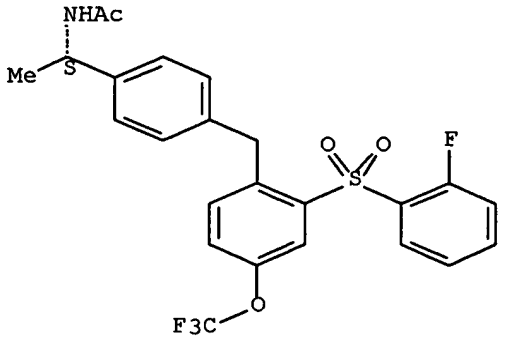
RN 447459-70-3 HCAPLUS
CN Benzenesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



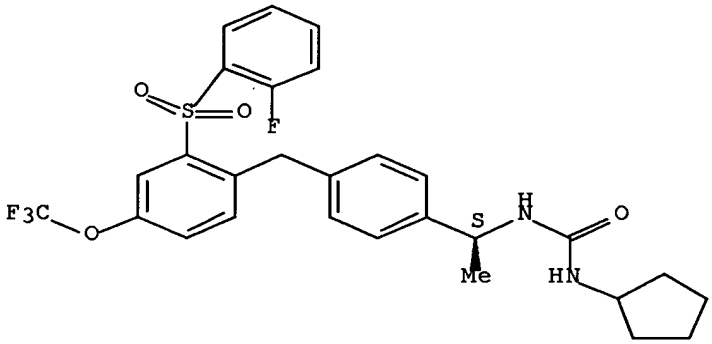
RN 447459-71-4 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



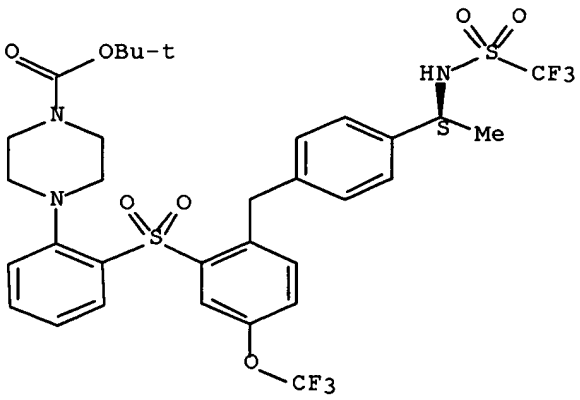
RN 447459-72-5 HCAPLUS
CN Urea, N-cyclopentyl-N'-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



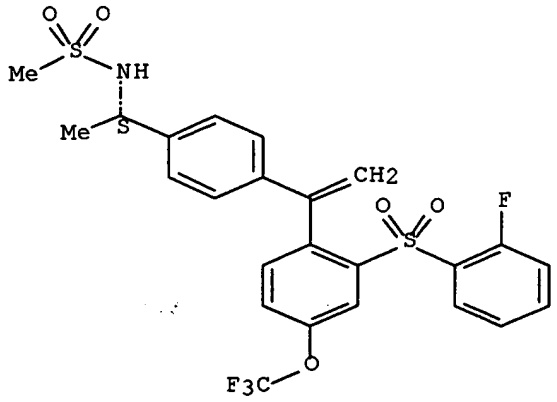
RN 447459-73-6 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[[5-(trifluoromethoxy)-2-[[4-[(1S)-1-[[(trifluoromethyl)sulfonyl]amino]ethyl]phenyl]methyl]phenyl]sulfonyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



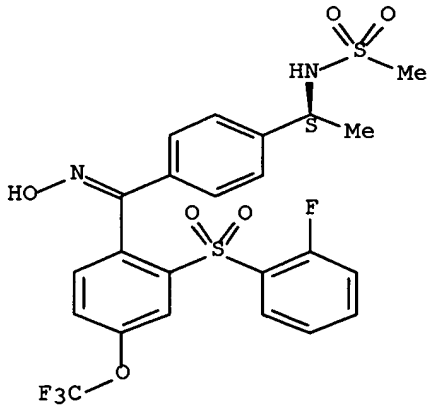
RN 447459-74-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[1-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]ethenyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



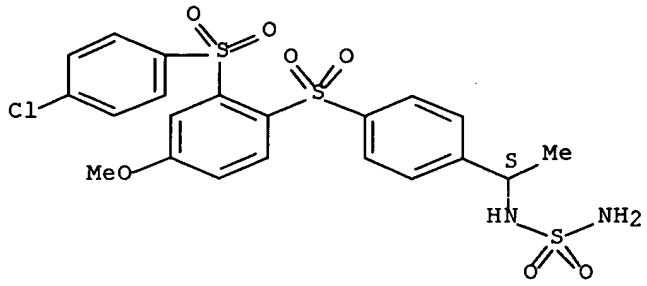
RN 447459-75-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl](hydroxyimino)methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

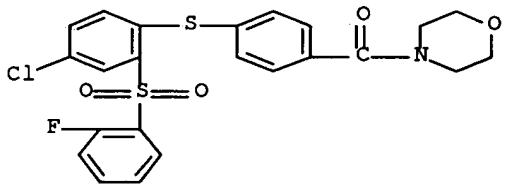


RN 447459-76-9 HCAPLUS
CN Sulfamide, [(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

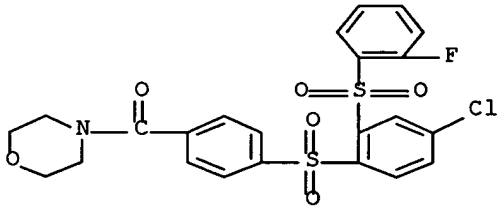
Absolute stereochemistry.



RN 447459-77-0 HCAPLUS
CN Morpholine, 4-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]thio]benzoyl]- (9CI) (CA INDEX NAME)

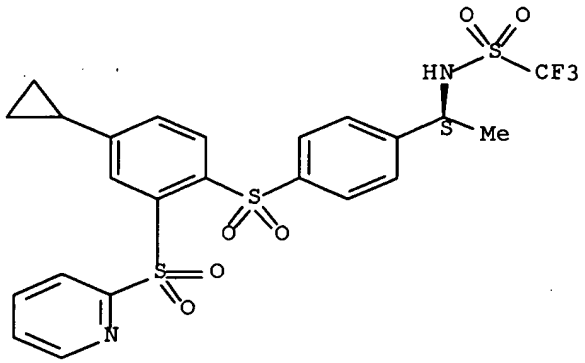


RN 447459-78-1 HCAPLUS
CN Morpholine, 4-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]benzoyl]- (9CI) (CA INDEX NAME)



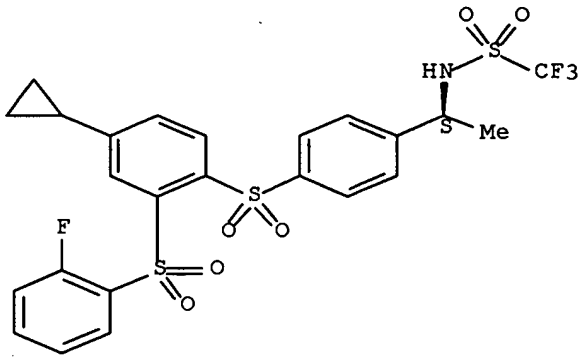
RN 447459-79-2 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



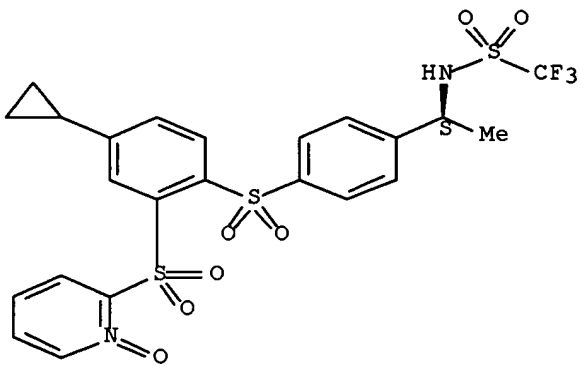
RN 447459-80-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



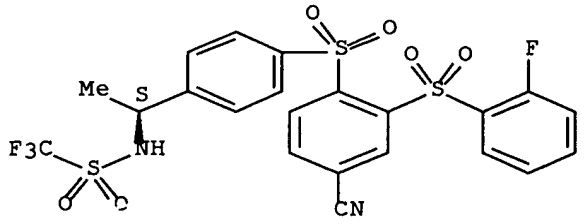
RN 447459-81-6 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-[(1-oxido-2-pyridinyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



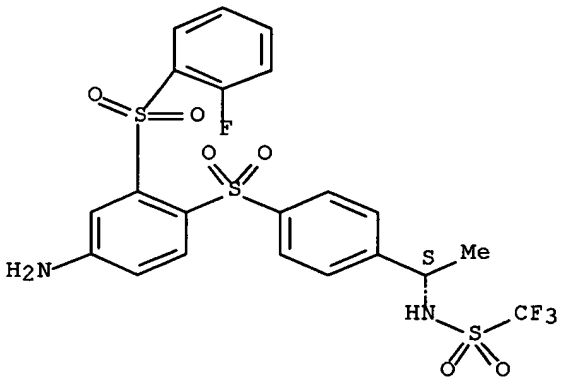
RN 447459-82-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyano-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



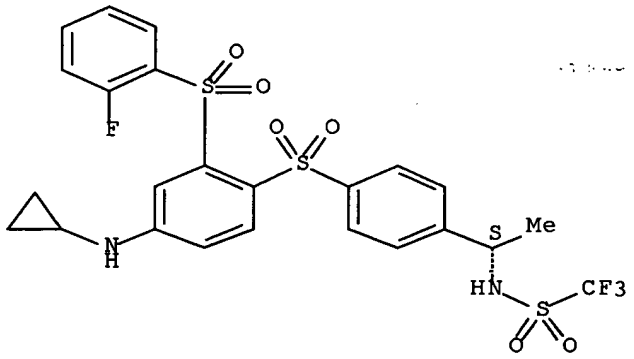
RN 447459-83-8 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-amino-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



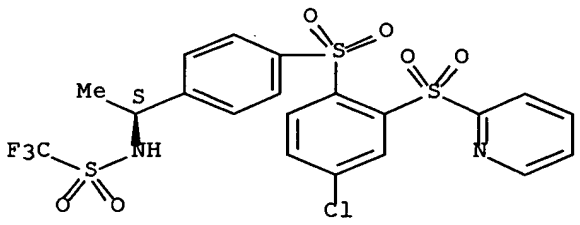
RN 447459-84-9 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-(cyclopropylamino)-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



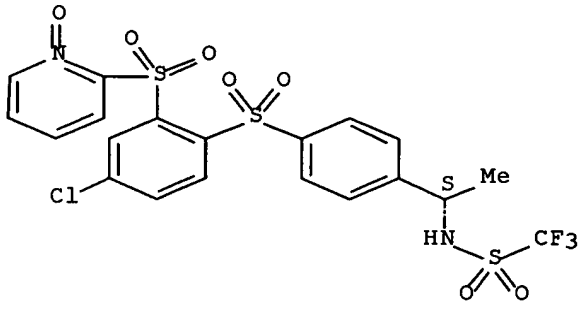
RN 447459-85-0 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



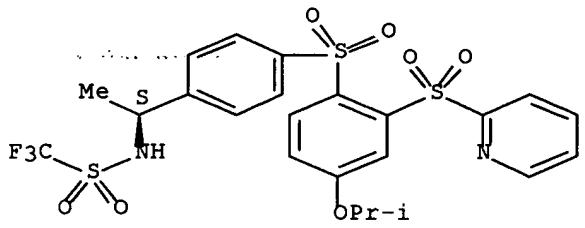
RN 447459-86-1 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-[(1-oxido-2-pyridinyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



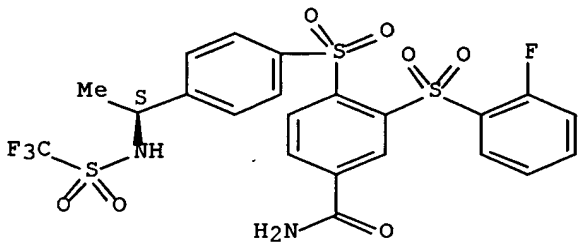
RN 447459-87-2 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[4-(1-methylethoxy)-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



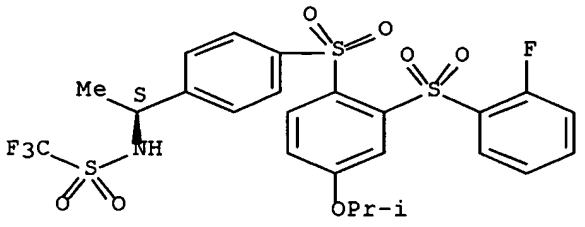
RN 447459-88-3 HCAPLUS
CN Benzamide, 3-[(2-fluorophenyl)sulfonyl]-4-[[4-[(1S)-1-[[(trifluoromethyl)sulfonyl]amino]ethyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



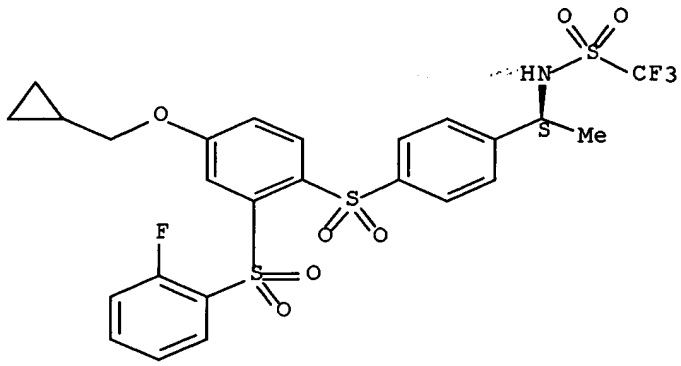
RN 447459-89-4 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(1-methylethoxy)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



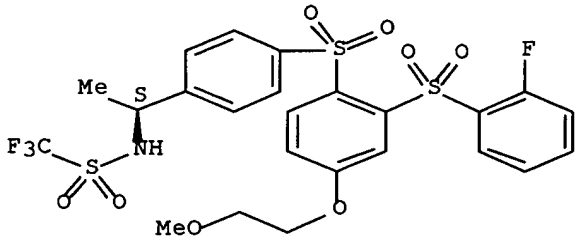
RN 447459-90-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-(cyclopropylmethoxy)-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



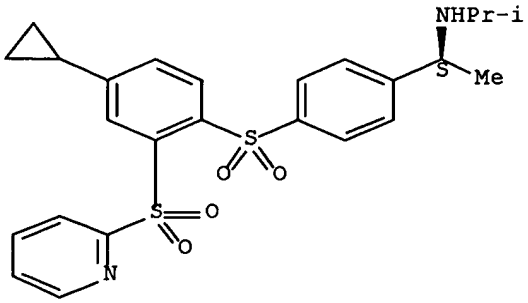
RN 447459-91-8 HCAPLUS
CN Methanesulfonamide, [illegible]-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(2-methoxyethoxy)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

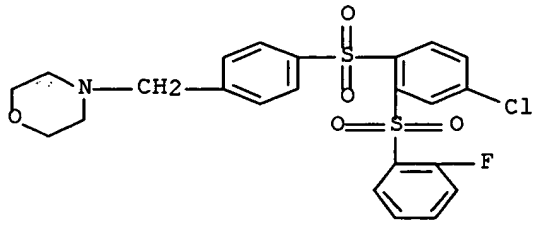


RN 447459-92-9 HCAPLUS
CN Benzenemethanamine, 4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-α-methyl-N-(1-methylethyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

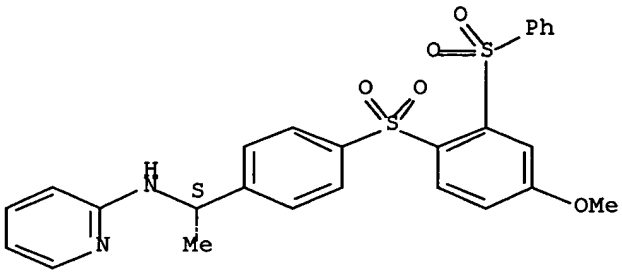


RN 447459-93-0 HCAPLUS
CN Morpholine, 4-[[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



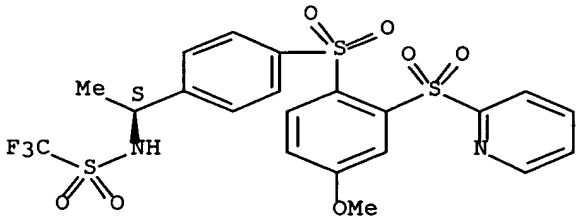
RN 447459-94-1 HCAPLUS
CN 2-Pyridinamine, N-[(1S)-1-[4-[[4-methoxy-2-(phenylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



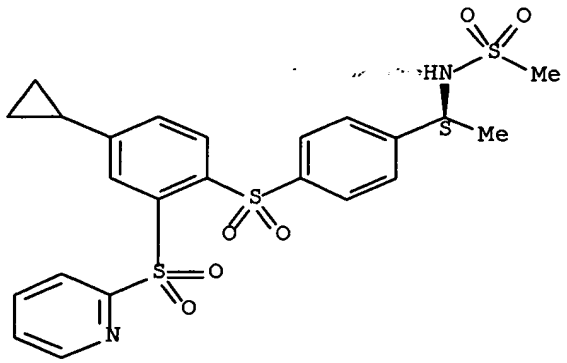
RN 447459-95-2 HCAPLUS
CN Methanesulfonamide, 1,1,1-trifluoro-N-[(1S)-1-[4-[[4-methoxy-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



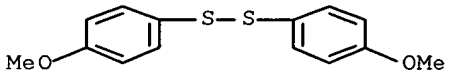
RN 447459-96-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

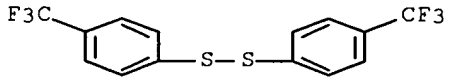


IT 5335-87-5, Bis(4-methoxyphenyl)disulfide 18715-45-2, Bis(4-trifluoromethylphenyl)disulfide 447460-46-0 447460-48-2 447460-49-3 447460-50-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of methylbenzylsulfonamides as cannabinoid receptor ligands)

RN 5335-87-5 HCAPLUS
CN Disulfide, bis(4-methoxyphenyl) (9CI) (CA INDEX NAME)

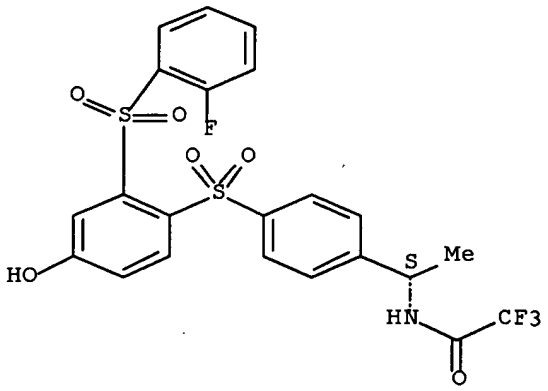


RN 18715-45-2 HCAPLUS
CN Disulfide, bis[4-(trifluoromethyl)phenyl] (9CI) (CA INDEX NAME)



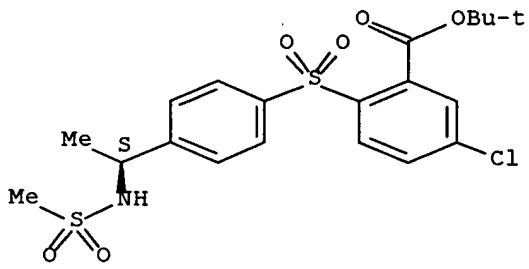
RN 447460-46-0 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-hydroxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



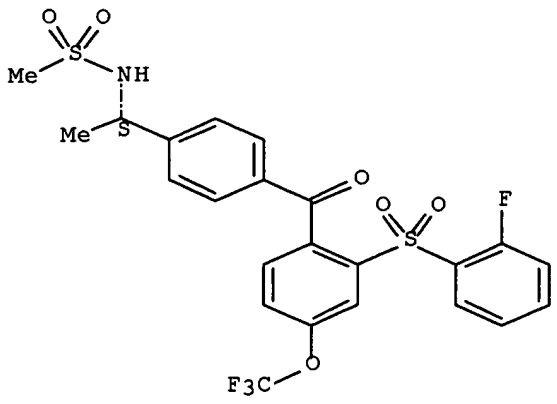
RN 447460-48-2 HCAPLUS
CN Benzoic acid, 5-chloro-2-[[4-[(1S)-1-[(methylsulfonyl)amino]ethyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 447460-49-3 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

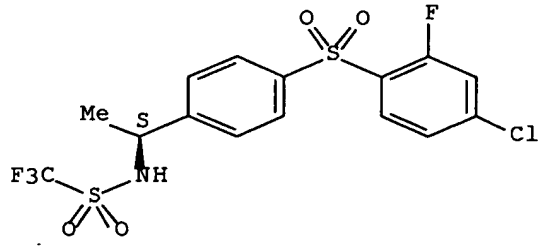
Absolute stereochemistry.



RN 447460-50-6 HCAPLUS

CN Methanesulfonamide, N-[(1S)-1-[4-[(4-chloro-2-fluorophenyl)sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 447459-97-4P 447459-98-5P 447459-99-6P
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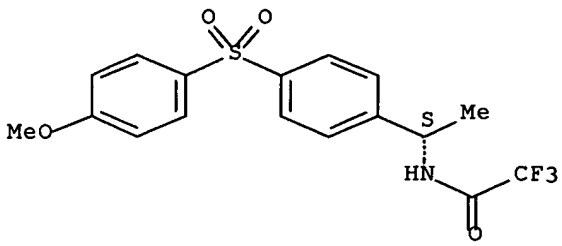
447460-42-6P 447460-44-8P 447460-45-9P
447460-47-1P 447460-51-7P 447460-52-8P
447460-53-9P 447460-54-0P 447460-69-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of methylbenzylsulfonamides as cannabinoid receptor ligands)

RN 447459-97-4 HCAPLUS

CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[(4-methoxyphenyl)sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

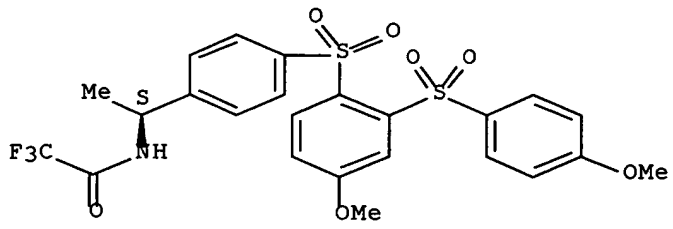


RN 447459-98-5 HCAPLUS

CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX

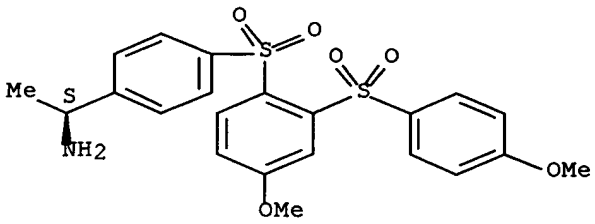
NAME)

Absolute stereochemistry.



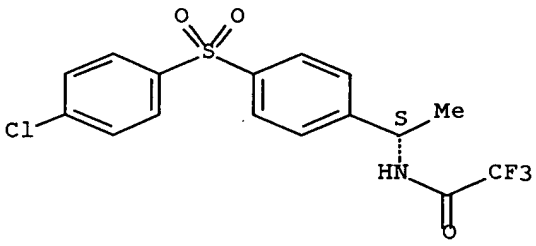
RN 447459-99-6 HCAPLUS
CN Benzenemethanamine, 4-[[4-methoxy-2-[(4-methoxyphenyl)sulfonyl]phenyl]sulf
onyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



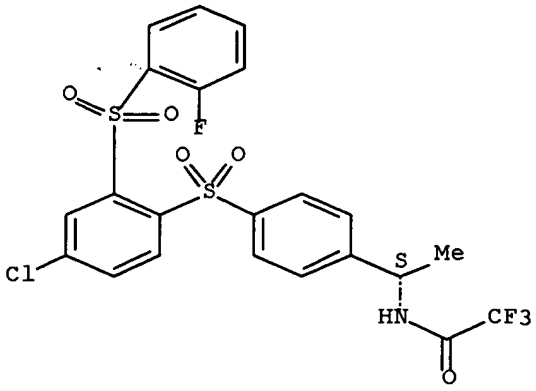
RN 447460-00-6 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chlorophenyl)sulfonyl]phenyl]ethyl]-2,2,2-
trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



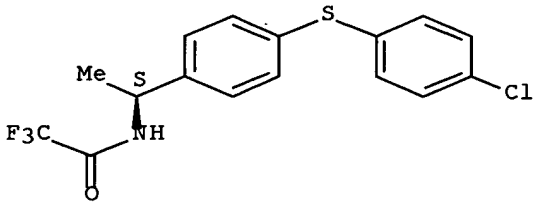
RN 447460-01-7 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulf
onyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



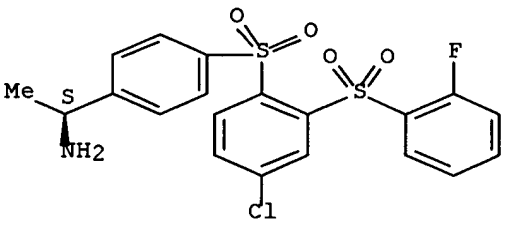
RN 447460-02-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chlorophenyl)thio]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



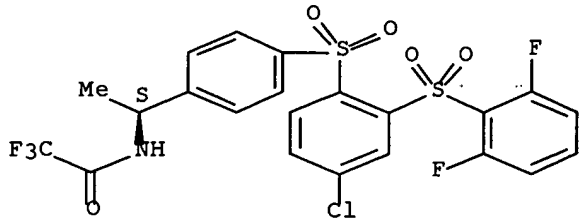
RN 447460-03-9 HCAPLUS
CN Benzenemethanamine, 4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



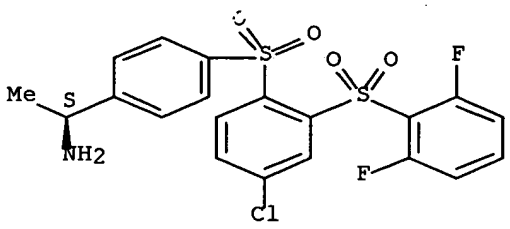
RN 447460-04-0 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

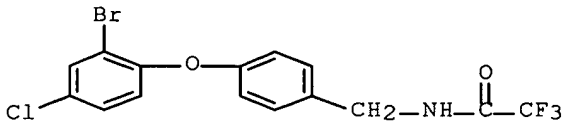


RN 447460-05-1 HCAPLUS
CN Benzenemethanamine, 4-[[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

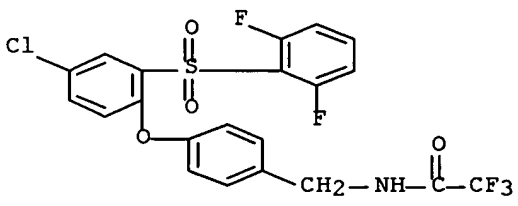
Absolute stereochemistry.



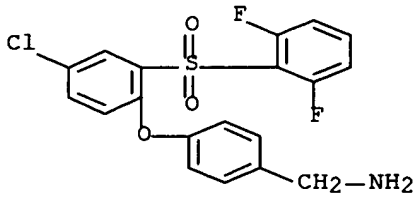
RN 447460-06-2 HCAPLUS
CN Acetamide, N-[[4-(2-bromo-4-chlorophenoxy)phenyl]methyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)



RN 447460-07-3 HCAPLUS
CN Acetamide, N-[[4-[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenoxy]phenyl]methyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

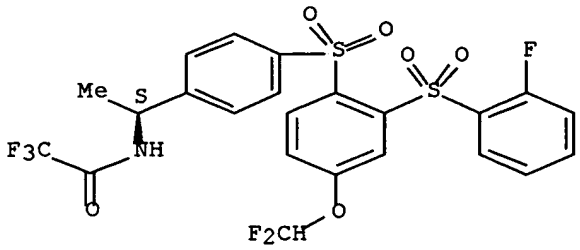


RN 447460-08-4 HCAPLUS
CN Benzenemethanamine, 4-[4-chloro-2-[(2,6-difluorophenyl)sulfonyl]phenoxy]- (9CI) (CA INDEX NAME)



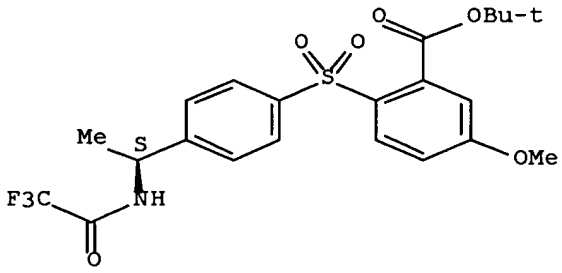
RN 447460-09-5 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-(difluoromethoxy)-2-[(2-fluorophenyl)sulfonyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



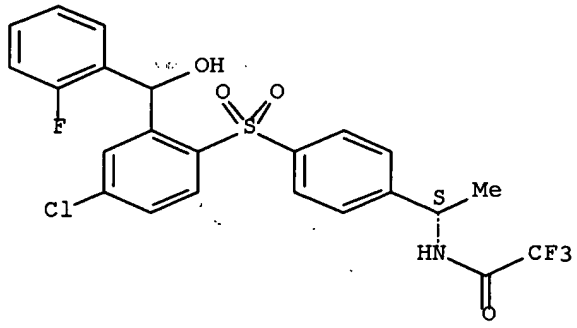
RN 447460-10-8 HCAPLUS
CN Benzoic acid, 5-methoxy-2-[[4-[(1S)-1-[(trifluoroacetyl)amino]ethyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



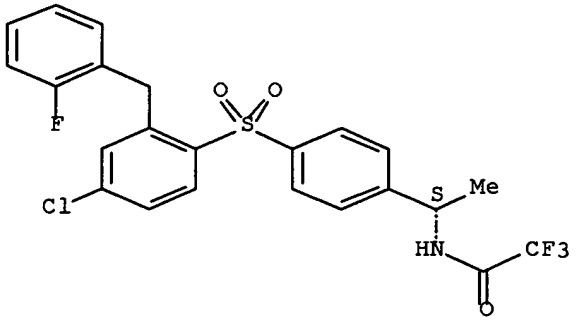
RN 447460-11-9 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)hydroxymethyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



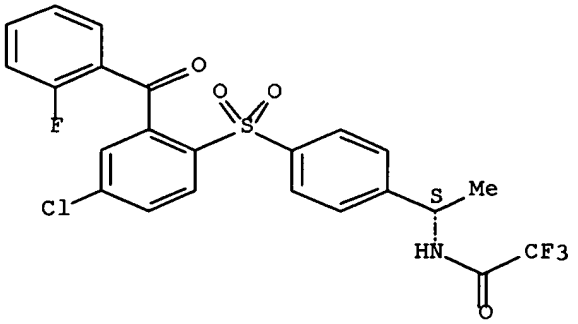
RN 447460-12-0 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(2-fluorophenyl)methyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



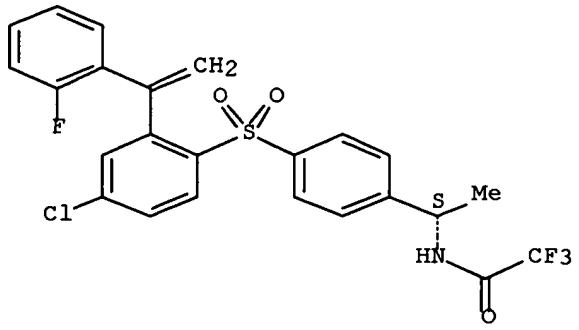
RN 447460-13-1 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-(2-fluorobenzoyl)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



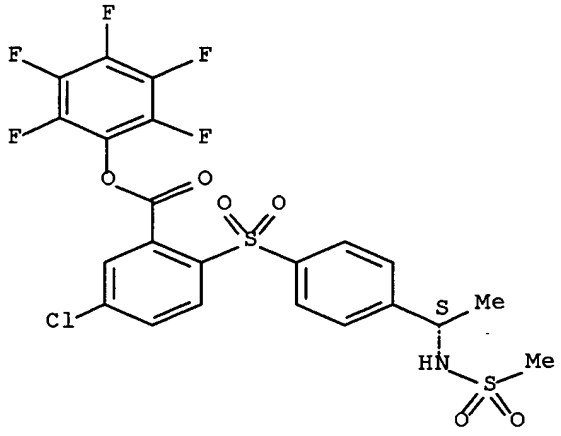
RN 447460-14-2 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[1-(2-fluorophenyl)ethenyl]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



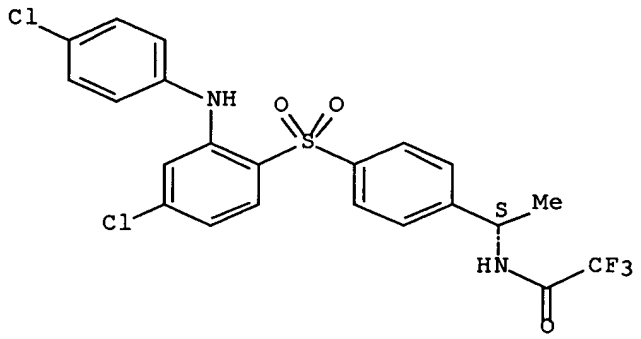
RN 447460-15-3 HCAPLUS
CN Benzoic acid, 5-chloro-2-[[4-[(1S)-1-[(methylsulfonyl)amino]ethyl]phenyl]sulfonyl]-, pentafluorophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



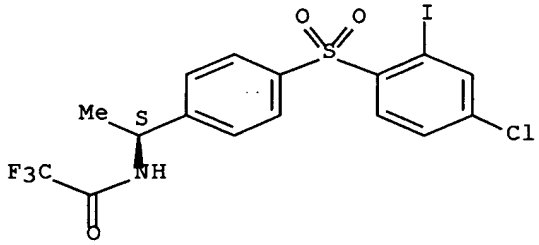
RN 447460-16-4 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-[(4-chlorophenyl)amino]phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



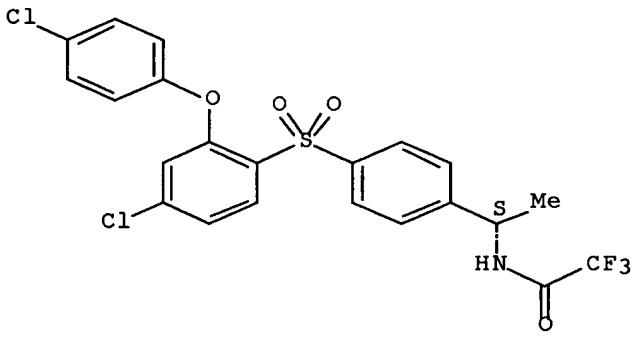
RN 447460-17-5 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chloro-2-iodophenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

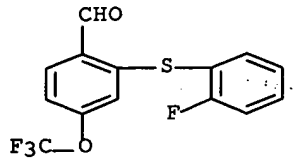


RN 447460-18-6 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-chloro-2-(4-chlorophenoxy)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

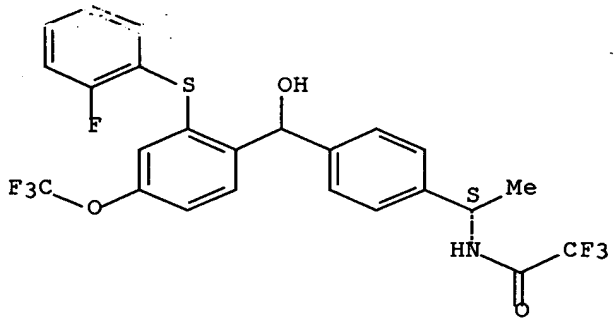


RN 447460-19-7 HCAPLUS
CN Benzaldehyde, 2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



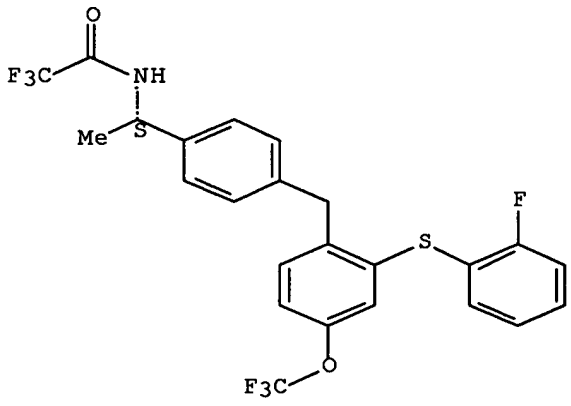
RN 447460-20-0 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)phenyl]hydroxymethyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



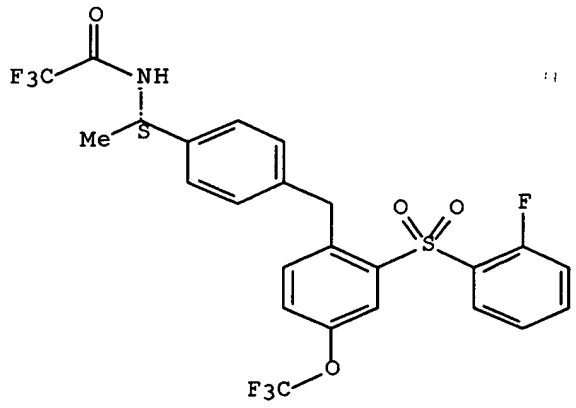
RN 447460-21-1 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



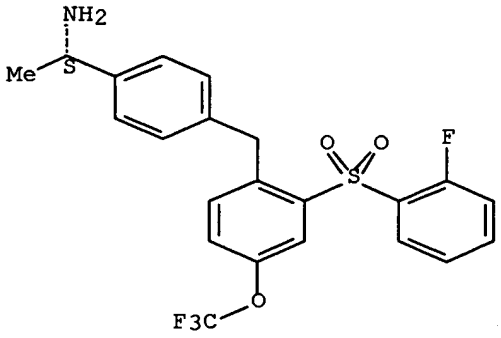
RN 447460-22-2 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



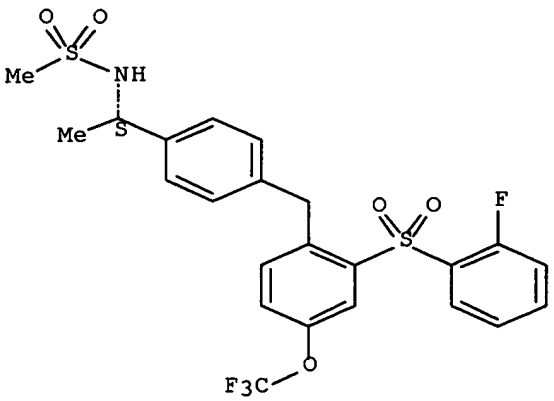
RN 447460-23-3 HCAPLUS
CN Benzenemethanamine, 4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



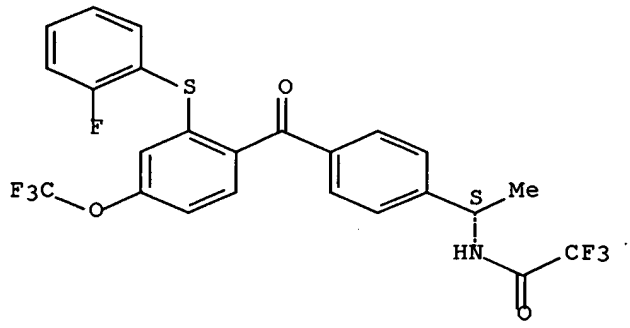
RN 447460-24-4 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



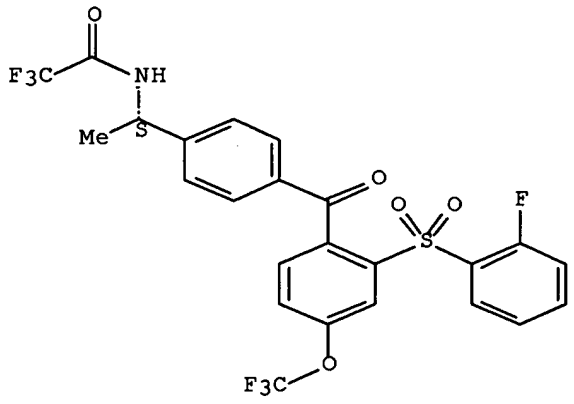
RN 447460-25-5 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[2-[(2-fluorophenyl)thio]-4-(trifluoromethoxy)benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



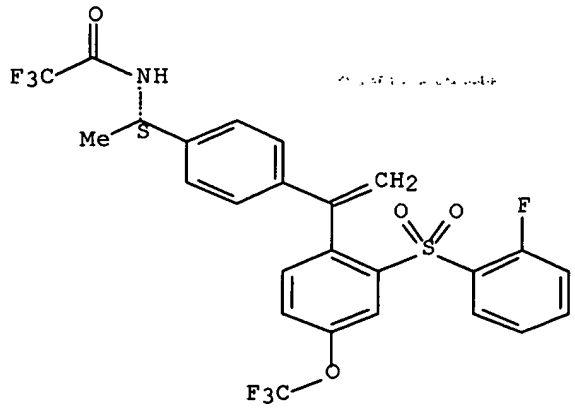
RN 447460-26-6 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)benzoyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



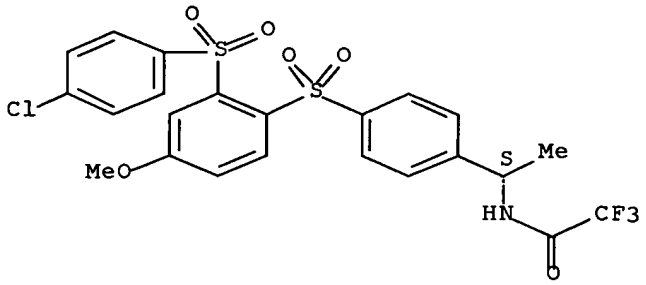
RN 447460-27-7 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[1-[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethoxy)phenyl]ethenyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



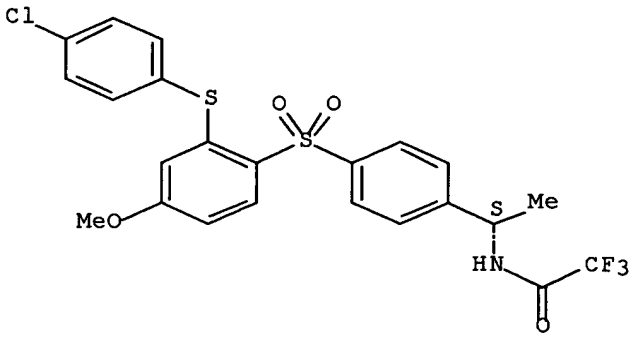
RN 447460-28-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



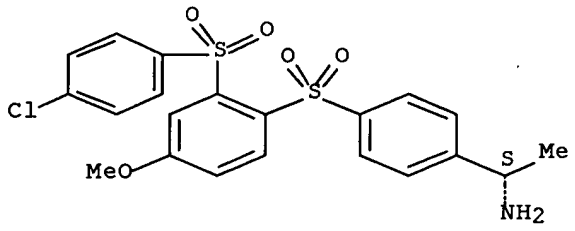
RN 447460-29-9 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[2-[(4-chlorophenyl)thio]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

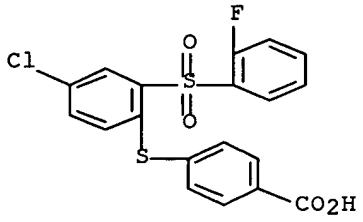


RN 447460-30-2 HCAPLUS
CN Benzenemethanamine, 4-[[2-[(4-chlorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

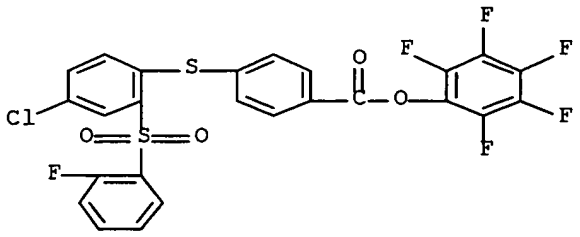
Absolute stereochemistry.



RN 447460-32-4 HCAPLUS
CN Benzoic acid, 4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]thio]- (9CI) (CA INDEX NAME)

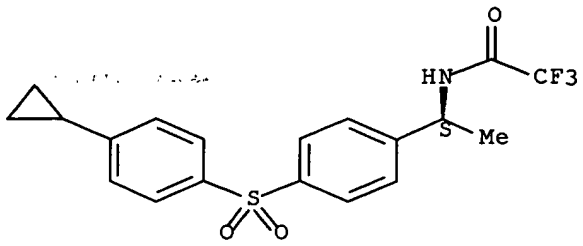


RN 447460-33-5 HCAPLUS
CN Benzoic acid, 4-[[4-chloro-2-[(2-fluorophenyl)sulfonyl]phenyl]thio]-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



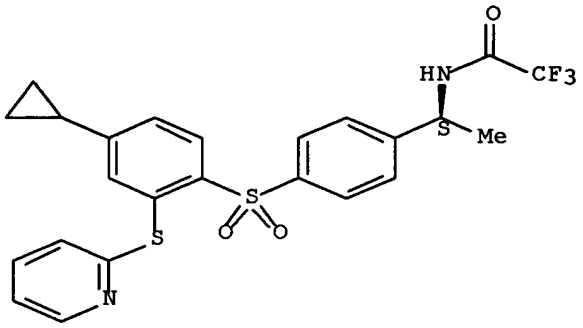
RN 447460-35-7 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-cyclopropylphenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



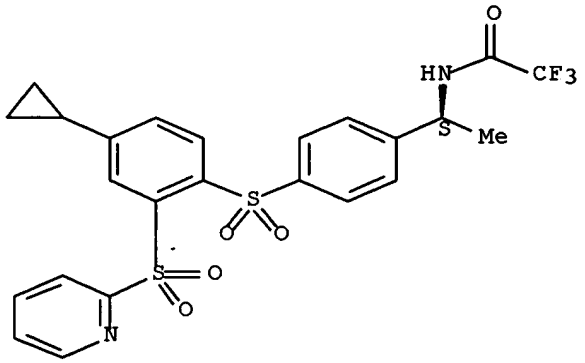
RN 447460-36-8 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-(2-pyridinylthio)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



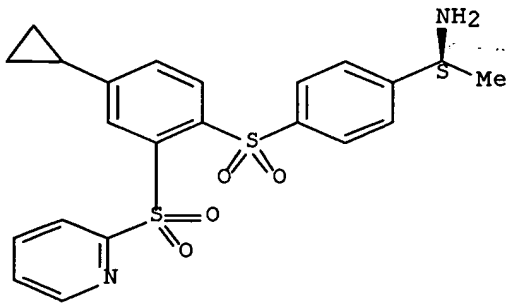
RN 447460-37-9 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



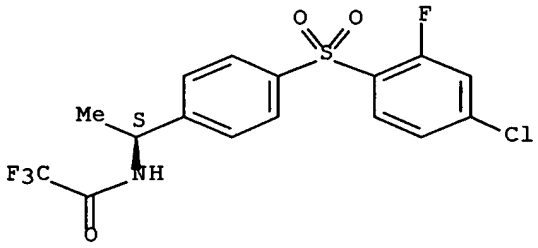
RN 447460-38-0 HCAPLUS
CN Benzenemethanamine, 4-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



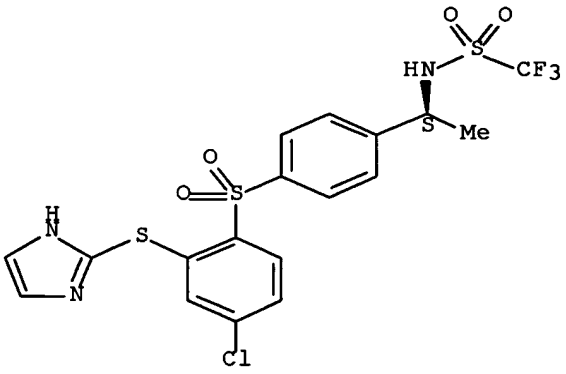
RN 447460-40-4 HCAPLUS
CN Acetamide, N-[(1S)-1-[4-[(4-chloro-2-fluorophenyl)sulfonyl]phenyl]ethyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



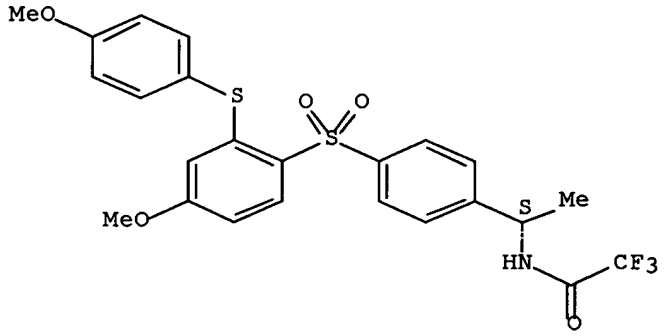
RN 447460-41-5 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[4-chloro-2-(1H-imidazol-2-ylthio)phenyl]sulfonyl]phenyl]ethyl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



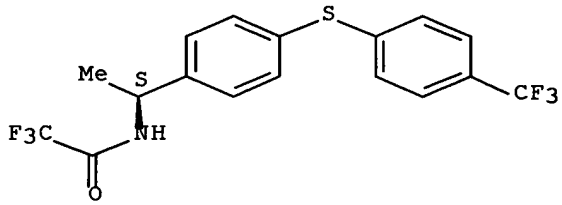
RN 447460-42-6 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[4-methoxy-2-[(4-methoxyphenyl)thio]phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



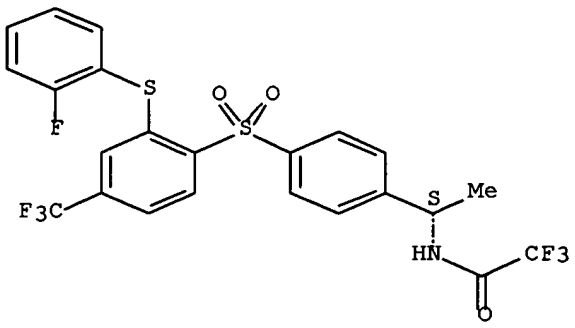
RN 447460-44-8 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[4-(trifluoromethyl)phenyl]thio]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



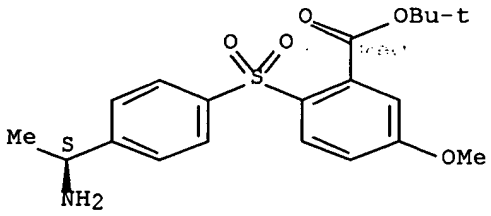
RN 447460-45-9 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)thio]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



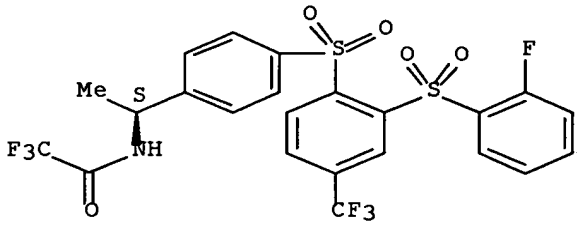
RN 447460-47-1 HCAPLUS
CN Benzoic acid, 2-[[4-[(1S)-1-aminoethyl]phenyl]sulfonyl]-5-methoxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



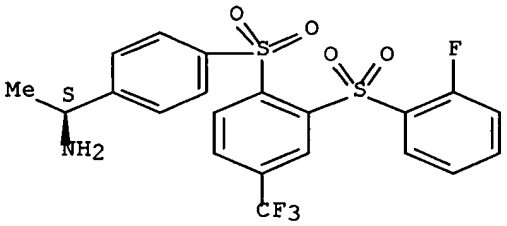
RN 447460-51-7 HCAPLUS
CN Acetamide, 2,2,2-trifluoro-N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

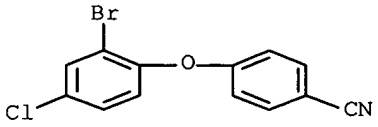


RN 447460-52-8 HCAPLUS
CN Benzenemethanamine, 4-[[2-[(2-fluorophenyl)sulfonyl]-4-(trifluoromethyl)phenyl]sulfonyl]-α-methyl-, (αS)- (9CI) (CA INDEX NAME)

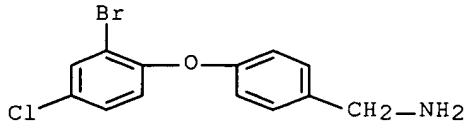
Absolute stereochemistry.



RN 447460-53-9 HCAPLUS
CN Benzonitrile, 4-(2-bromo-4-chlorophenoxy)- (9CI) (CA INDEX NAME)

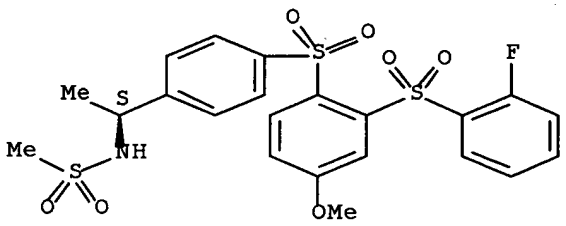


RN 447460-54-0 HCAPLUS
CN Benzenemethanamine, 4-(2-bromo-4-chlorophenoxy)- (9CI) (CA INDEX NAME)



RN 447460-69-7 HCAPLUS
CN Methanesulfonamide, N-[(1S)-1-[4-[[2-[(2-fluorophenyl)sulfonyl]-4-methoxyphenyl]sulfonyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 34 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:611311 HCAPLUS Full-text
DOCUMENT NUMBER: 137:184205
TITLE: High levels of osteoprotegerin and soluble receptor activator of nuclear factor .vkappa.B ligand in serum of rheumatoid arthritis patients and their normalization after anti-tumor necrosis factor α treatment
AUTHOR(S): Ziolkowska, Maria; Kurowska, Mariola; Radzikowska, Anna; Luszczykiewicz, Grazyna; Wiland, Piotr; Dziewczopolski, Wojciech; Filipowicz-Sosnowska, Anna; Pazdur, Jacek; Szechinski, Jacek; Kowalczewski, Jacek; Rell-Bakalarska, Maria; Maslinski, Wlodzimierz
CORPORATE SOURCE: Institute of Rheumatology, Warsaw, Pol.
SOURCE: Arthritis & Rheumatism (2002), 46(7), 1744-1753
CODEN: ARHEAW; ISSN: 0004-3591
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The aim of this study was to test the hypotheses that (1) proinflammatory cytokines affect osteoprotegerin (OPG) and soluble receptor activator of nuclear factor .vkappa.B ligand (sRANKL) production and therefore the OPG and sRANKL levels differ in rheumatoid arthritis (RA) patients in comparison with healthy individuals; and (2) anti-tumor necrosis factor α (anti-TNFα) therapy influences OPG and sRANKL levels. Sera were obtained from healthy individuals or RA patients receiving the combination of infliximab and methotrexate. Peripheral blood mononuclear cells (PBMCs) and synovial fluid mononuclear cells (SFMCs) were isolated from RA patients. Fibroblast-like synoviocytes

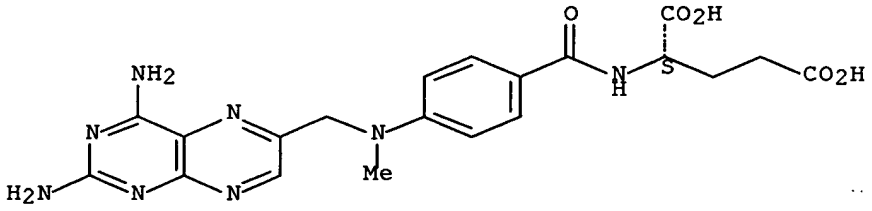
(FLS) were isolated from synovial tissue obtained at total knee replacement in RA patients. Supernatants from cells stimulated with cytokines were collected after culture in vitro. Concns. of OPG and sRANKL were determined by enzyme-linked immunosorbent assays. A strong pos. correlation between OPG concentration and age was observed in healthy individuals but not in RA patients. The OPG and sRANKL levels were higher in RA patients than in healthy controls. Cultured FLS spontaneously secreted much higher amts. of OPG than PBMCs or SFMCs. Proinflammatory cytokines enhanced OPG production Anti-TNFα treatment resulted in the normalization of serum OPG and sRANKL levels in RA patients without influencing the OPG:sRANKL ratio. Although higher serum levels of OPG and sRANKL are present in RA patients than in healthy individuals, the ratio of OPG:sRANKL is similar. There is an age-dependent increase of OPG but not sRANKL levels in healthy subjects. Anti-TNFα treatment results in the normalization of elevated levels of OPG and sRANKL in RA patients.

IT 59-05-2, Methotrexate
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(high levels of osteoprotegerin and soluble receptor activator of nuclear factor .vkappa.B ligand in serum of rheumatoid arthritis patients and normalization after anti-tumor necrosis factor α treatment)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 35 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:31914 HCAPLUS Full-text
DOCUMENT NUMBER: 136:98820
TITLE: Yeast three-hybrid system for in vivo drug screening and enzyme evolution using chemical inducers of dimerization
INVENTOR(S): Cornish, Virginia W.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 48 pp., Cont.-in-part of U.S. Ser. No. 490,320.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 2002004202	A1	20020110	US 2001-768479	20010124
US 2004106154	A1	20040603	US 2003-705644	20031110
PRIORITY APPLN. INFO.:			US 2000-490320	A2 20000124
			US 2001-768479	A3 20010124

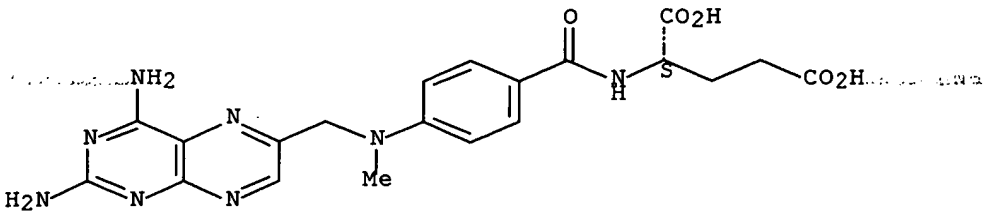
AB The disclosed invention relates to the evolution of enzymes in vivo, and drug screening in vivo through the use of chemical inducers of protein dimerization. The subject invention provides a compound having the formula: H1--X--B-Y--H2 wherein each of H1 and H2 may be the same or different and capable of binding to a receptor which is the same or different; wherein each of X and Y may be present or absent and if present, each may be the same or different spacer moiety; and wherein B is an enzyme cleavable moiety. This invention also provides a method of screening proteins for the ability to catalyze bond cleavage or bond formation, comprising the steps of: (a) providing a cell that expresses a pair of fusion proteins which upon dimerization change a cellular readout; (b) providing the compound of the invention which dimerizes the pair of fusion proteins, said compound comprising two portions coupled by a bond that is cleavable or formed by the protein to be screened; and (c) screening for the cellular readout, wherein a change the cellular readout indicates catalysis of bond cleavage or bond formation by the protein to be screened. However, it has not heretofore been suggested to use small mol. induced protein dimerization to screen for catalysis in vivo., and specifically, it has not been suggested to use an enzyme cleavable moiety to link two mols. to dimerize proteins. This invention provides proteins de novo with prescribed binding and catalytic properties and permits screening cDNA libraries based on biochem. function. Practically, we believe that powerful screens in combination with existing randomization techniques will make it possible to take an existing protein fold and evolve it into an enzyme with a new function generating useful catalysts for the pharmaceutical and chemical industries. Since the screen is done in vivo and in both prokaryotes and eukaryotes, the methodol. can be applied to functional genomics and drug discovery. A new chemical inducer of dimerization (CID) was recently developed in Professor Cornish's lab, which uses a heterodimer of methotrexate (MTX) and dexamethasone (DEX) which, when placed in the yeast three-hybrid system, reconstitutes transcription of the lacZ gene. The effects of altering the structure of the DEX-MTX CID and the protein chimeras in the three-hybrid assay were investigated. It was observed that all DEX-MTX CIDs, except the DEX-MTX CID with the shortest chemical linker, showed the ability to induce β-galactosidase levels at levels 400% above strains possessing no CID. The DEX-MTX CIDs showed little or no increase in β-galactosidase levels above background levels in strains where dihydrofolate reductase (DHFR) from E. coli was replaced by DHFR from murine. The three-hybrid system did show some directional preference to the way in which the receptors where fused to the DNA binding domain and the activation domain. These studies have led to a better understanding of the factors that are important in activating transcription in the DEX-MTX yeast three-hybrid system.

IT 59-05-2D, Methotrexate, conjugates with receptor ligands
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(yeast three-hybrid system for in vivo drug screening and enzyme evolution using chemical inducers of dimerization)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 36 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:731094 HCAPLUS Full-text
DOCUMENT NUMBER: 135:285352
TITLE: Compositions and methods using GCC for identifying and targeting cancer cells of alimentary canal origin
INVENTOR(S): Waldman, Scott A.; Park, Jason; Schulz, Stephanie
PATENT ASSIGNEE(S): Thomas Jefferson University, USA
SOURCE: PCT Int. Appl., 89 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001073132	A1	20011004	WO 2001-US9790	20010327
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2404431	AA	20011004	CA 2001-2404431	20010327
AU 2001049504	A5	20011008	AU 2001-49504	20010327
US 2001029019	A1	20011011	US 2001-819249	20010327
US 6767704	B2	20040727		
US 2001029020	A1	20011011	US 2001-819254	20010327
US 2001036635	A1	20011101	US 2001-819247	20010327
US 2001039016	A1	20011108	US 2001-819248	20010327
US 2001039017	A1	20011108	US 2001-819252	20010327
US 6844153	B2	20050118		
US 2002012931	A1	20020131	US 2001-820215	20010327
EP 1272665	A1	20030108	EP 2001-922739	20010327
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003528628	T2	20030930	JP 2001-570845	20010327
US 2004033520	A1	20040219	US 2003-428225	20030502
US 2005059008	A1	20050317	US 2003-611533	20030630
US 2004224355	A1	20041111	US 2004-866951	20040614
US 2005164267	A1	20050728	US 2005-36875	20050114
US 2005196793	A1	20050908	US 2005-58778	20050216
PRIORITY APPLN. INFO.:			US 2000-192229P	P 20000327
			US 2001-819247	B1 20010327
			US 2001-819249	A3 20010327

US 2001-819252	A3	20010327
US 2001-819254	B1	20010327
WO 2001-US9790	W	20010327
US 2005-36875	A1	20050114

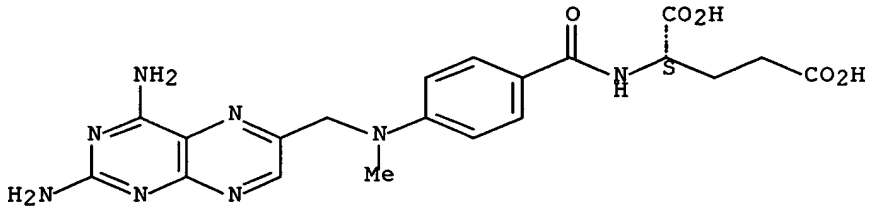
AB Screening and diagnostic reagents, kits and methods for primary and/or metastatic stomach or esophageal cancer are disclosed. Compns. for and methods of imaging and treating primary and/or metastatic stomach or esophageal cancer are disclosed. Vaccines compns. and methods for treating and preventing primary and/or metastatic stomach or esophageal cancer are disclosed. GCC or its gene transcript is determined by immunoassay or by PCR.

IT 59-05-2D, Methotrexate, conjugates with ST receptor ligand
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. and methods using GCC for identifying and targeting cancer cells of alimentary canal origin)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 37 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2001:519065 HCAPLUS Full-text
DOCUMENT NUMBER:	135:340580
TITLE:	Sensitivity of an empirical affinity scoring function to changes in receptor-ligand complex conformations
AUTHOR(S):	Marelius, J.; Ljungberg, K. B.; Aqvist, J.
CORPORATE SOURCE:	Department of Cell and Molecular Biology, Uppsala University, Uppsala, SE-751 24, Swed.
SOURCE:	European Journal of Pharmaceutical Sciences (2001), 14(1), 87-95 CODEN: EPSCED; ISSN: 0928-0987
PUBLISHER:	Elsevier Science Ireland Ltd.
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB A combination of empirical scoring and conformational sampling for ligand binding affinity prediction is examined The behavior of a scoring function with respect to the sensitivity to conformational changes is investigated using ensembles of structures generated by mol. dynamics simulation. The correlation between the calculated score and the coordinate deviation from the exptl. structure is clear for the complex of arabinose with arabinose-binding protein, which is dominated by hydrogen bond interactions, while the score calculated for the hydrophobic complex between retinol and retinol binding protein is rather insensitive to ligand conformational changes. For typical ensembles of structures generated by mol. dynamics at 300 K, the variation of

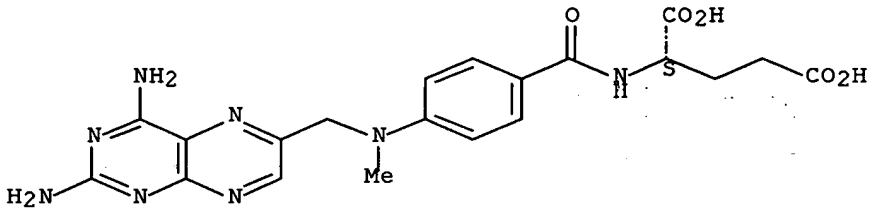
the calculated score is considerably smaller than that of the underlying mol. mechanics interaction energies.

IT 59-05-2, Methotrexate
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(sensitivity of an empirical affinity scoring function to changes in receptor-ligand complex conformations)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 38 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:137880 HCAPLUS Full-text
DOCUMENT NUMBER: 134:320522
TITLE: SLATE: a method for the superposition of flexible ligands
AUTHOR(S): Mills, J. E. J.; De Esch, I. J. P.; Perkins, T. D. J.; Dean, P. M.
CORPORATE SOURCE: Drug Design Group, Department of Pharmacology, University of Cambridge, Cambridge, CB2 IQJ, UK
SOURCE: Journal of Computer-Aided Molecular Design (2001), 15(1), 81-96
CODEN: JCADEQ; ISSN: 0920-654X
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel program for the superposition of flexible mols., SLATE, is presented. It uses simulated annealing to minimize the difference between the distance matrixes calculated from the hydrogen-bonding and aromatic ring properties of two ligands. A method for generating a mol. stack using multiple pairwise matches is illustrated. These stacks are used by the program DOH to predict the relative positions of receptor atoms that could form hydrogen bonds to two or more ligands in the dataset. The methodol. has been applied to ligands binding to dihydrofolate reductase, thermolysin, H3 histamine receptors, α2 adrenoceptors and 5-HT1D receptors. When there are sufficient nos. and diversity of mols. in the dataset, the prediction of receptor-atom positions is applicable to compound design.

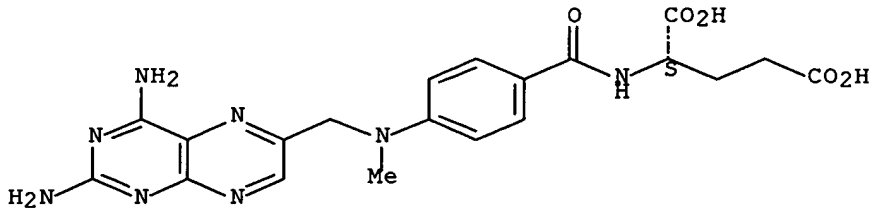
IT 59-05-2, Methotrexate
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(SLATE method for superposition of flexible ligands: application to ligands binding to dihydrofolate reductase,

thermolysin, H3 histamine receptors, α2 adrenoceptors and 5-HT1D receptors)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 39 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:207165 HCAPLUS Full-text

DOCUMENT NUMBER: 133:83972

TITLE: Drug-induced apoptosis in osteosarcoma cell lines is mediated by caspase activation independent of CD95-receptor/ligand interaction

AUTHOR(S): Fellenberg, J.; Mau, H.; Nedel, S.; Ewerbeck, V.; Debatin, K-M.

CORPORATE SOURCE: Stiftung Orthopadische Universitatsklinik Heidelberg, Heidelberg, 69118, Germany

SOURCE: Journal of Orthopaedic Research (2000), 18(1), 10-17
CODEN: JOREDR; ISSN: 0736-0266

PUBLISHER: Journal of Bone and Joint Surgery, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

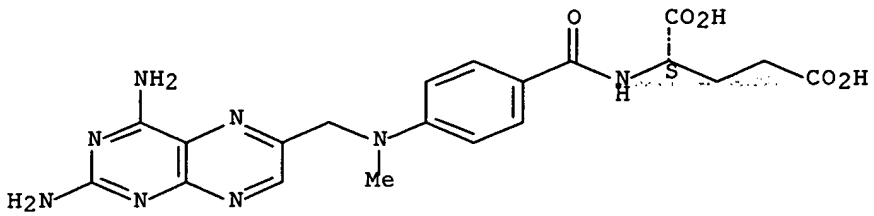
AB Cytotoxic drugs (doxorubicin, methotrexate, cisplatin) induced biochem. and morphol. alterations characteristic of apoptosis in osteosarcoma cell lines, including activation of caspases and disturbance of mitochondrial function. However, drug treatment did not result in activation of CD95-receptor or CD95-ligand mRNA. In addition, drug-induced apoptosis was blocked by caspase inhibitors but not by inhibition of CD95-ligand action, indicating a CD95-receptor/ligand-independent mechanism in osteosarcoma cell lines.

IT 59-05-2, Methotrexate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(drug-induced apoptosis in osteosarcoma cell lines mediated by caspase activation independently of CD95-receptor/ligand interaction)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 40 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:2517 HCAPLUS Full-text
DOCUMENT NUMBER: 132:106828
TITLE: Ligand-activation of the adenosine A2a receptors inhibits IL-12 production by human monocytes
AUTHOR(S): Link, Amrey A.; Kino, Tomoshige; Worth, James A.; McGuire, Jennifer L.; Crane, Marianna L.; Chrousos, George P.; Wilder, Ronald L.; Elenkov, Ilia J.
CORPORATE SOURCE: Developmental Endocrinology Branch, National Institute of Child Health and Human Development, National Institutes of Health, Bethesda, MD, 20892, USA
SOURCE: Journal of Immunology (2000), 164(1), 436-442
CODEN: JOIMA3; ISSN: 0022-1767
PUBLISHER: American Association of Immunologists
DOCUMENT TYPE: Journal
LANGUAGE: English

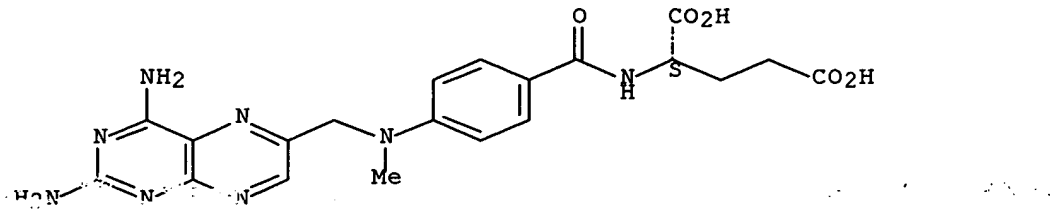
AB Adenosine (ADO) exerts potent anti-inflammatory and immunosuppressive effects. In this paper we address the possibility that these effects are partly mediated by inhibition of the secretion of IL-12, a proinflammatory cytokine and a major inducer of Th1 responses. We demonstrate that 5'-N-ethylcarboxamidoadenosine (NECA), a nonspecific ADO analog, and 2-p-(2-carbonylethyl)phenylethylamino-5'-N-ethylcarboxamidoadenosine (CGS-21680), a specific A2a receptor agonist, dose-dependently inhibited, in whole blood ex vivo and monocyte cultures, the production of human IL-12 induced by LPS and Staphylococcus aureus Cowan strain 1. However, the A1 receptor agonist 2-chloro-N6-cyclopentyladenosine and the A3 receptor agonists N6-benzyl-NECA and 1-deoxy-1-[6-[[(3-iodophenyl)methyl]amino]-9H- purin-9-yl]-N-methyl-β-D-ribofuranuronamide expressed only weak inhibitory effects. On the other hand, NECA and CGS-21680 dose-dependently potentiated the production of IL-10. The differential effect of these drugs on monocyte IL-12 and IL-10 production implies that these effects are mediated by A2a receptor signaling rather than by intracellular toxicity of ADO analog's metabolites. Moreover, CGS-21680 inhibited IL-12 production independently of endogenous IL-10 induction, because anti-IL-10 Abs failed to prevent its effect. The selective A2a antagonist 8-(3-chlorostyryl) caffeine prevented the inhibitory effect of CGS-21680 on IL-12 production The phosphodiesterase inhibitor Ro 20-1724 dose-dependently potentiated the inhibitory effect of CGS-21680 and, furthermore, Rp-cAMPS, a protein kinase A inhibitor, reversed the inhibitory effect of CGS-21680, implicating a cAMP/protein kinase A pathway in its action. Thus, ligand activation of A2a receptors simultaneously inhibits IL-12 and stimulates IL-10 production by human monocytes. Through this mechanism, ADO released in excess during inflammatory and ischemic conditions, or tissue injury, may contribute to selective suppression of Th1 responses and cellular immunity.

IT 59-05-2, Methotrexate 599-79-1, Sulfasalazine

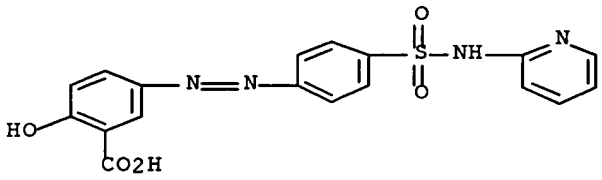
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ligand-activation of adenosine A2a receptors
inhibits interleukin 12 production by human monocytes in relation to
treatment with)

RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzo
yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 599-79-1 HCAPLUS
CN Benzoic acid, 2-hydroxy-5-[[4-[(2-pyridinylamino)sulfonyl]phenyl]azo]-
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 41 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:705037 HCAPLUS Full-text
DOCUMENT NUMBER: 131:341963
TITLE: Fusion proteins comprising brain capillary endothelial cell receptor ligands with neuropharmaceutical agents for delivery across the blood-brain barrier
INVENTOR(S): Friden, Phillip M.; Starzyk, Ruth M.; Morrison, Sherie L.; Park, Eun Chung; McGrath, John P.
PATENT ASSIGNEE(S): Alkermes Inc., USA; The Regents of the University of California
SOURCE: U.S., 43 pp., Cont.-in-part of U.S. 5,672,683.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5977307	A	19991102	US 1996-581543	19960213
US 5154924	A	19921013	US 1989-404089	19890907

CA 2066244		AA	19910308	CA 1990-2066244	19900907
WO 9103259		A1	19910321	WO 1990-US5077	19900907
W:	AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU, US				
RW:	AT, BE, BF, BJ, CF, CG, CH, CM, DE, DK, ES, FR, GA, GB, IT, LU, ML, MR, NL, SE, SN, TD, TG				
AU 9064459		A1	19910408	AU 1990-64459	19900907
AU 654115		B2	19941027		
EP 490998		A1	19920624	EP 1990-914638	19900907
EP 490998		B1	19951206		
R:	AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
JP 05500944		T2	19930225	JP 1990-513735	19900907
AT 131070		E	19951215	AT 1990-914638	19900907
ES 2080838		T3	19960216	ES 1990-914638	19900907
US 5182107		A	19930126	US 1992-846830	19920306
US 5527527		A	19960618	US 1993-4986	19930115
US 5672683		A	19970930	US 1993-94534	19930716
WO 9521245		A1	19950810	WO 1995-US1469	19950203
W:	AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US				
RW:	KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5833988		A	19981110	US 1996-634328	19960418
PRIORITY APPLN. INFO.:				US 1989-404089	A2 19890907
				WO 1990-US5077	A2 19900907
				US 1992-846830	A3 19920306
				US 1992-999803	B2 19921120
				US 1993-94534	A2 19930716
				WO 1995-US1469	W 19950203
				US 1993-4986	A1 19930115
				US 1994-192288	A2 19940203

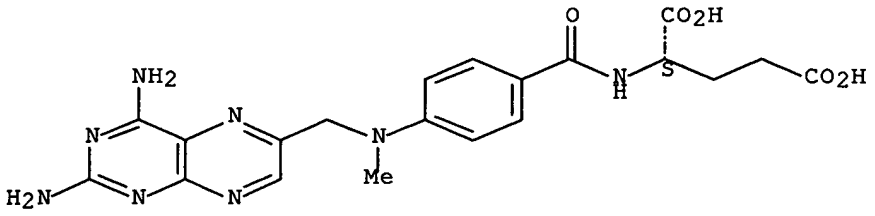
AB The present invention pertains to a method for delivering a neuropharmaceutical agent across the blood brain barrier to the brain of a host. The method comprises administering to the host a therapeutically effective amount of a ligand-neuropharmaceutical agent fusion protein wherein the ligand is reactive with a brain capillary endothelial cell receptor. Anti-(transferrin receptor) antibody conjugates with a neuropharmaceutical or a diagnostic agent are prepared for delivering the neuropharmaceutical or diagnostic agent across the blood-brain barrier to the brain of a subject. The antibody is a chimera between the variable region of a murine antibody and the constant region of a sep. antibody (e.g. that of a human antibody). Mouse anti-(rat transferrin receptor) monoclonal antibody OX-26 was conjugated to peroxidase, adriamycin, methotrexate, AZT, or soluble CD4; each conjugate crossed the blood-brain barrier. Brain capillary endothelial cell receptor ligands may comprise transferrin or the anti-(transferrin receptor) antibody, insulin or the anti-(insulin receptor) antibody, or antibodies to the receptors for insulin-like growth factor-1 and -2. The neuropharmaceutical agents are selected from nerve growth factor, ciliary neurotrophic factor, growth factors, superoxide dismutase, CD4, lymphokines, lymphokine antagonists, cytokine antagonists, dopamine decarboxylase, and trichosanthin.

IT 59-05-2, Methotrexate
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fusion proteins comprising brain capillary endothelial cell receptor ligands with neuropharmaceutical agents for delivery across the blood-brain barrier)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

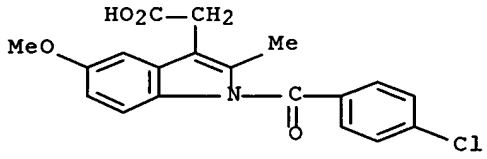
L21 ANSWER 42 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:518102 HCAPLUS Full-text
DOCUMENT NUMBER: 129:239579
TITLE: Ligand for peroxisome proliferator-activated receptor γ (troglitazone) has potent antitumor effect against human prostate cancer both in vitro and in vivo
AUTHOR(S): Kubota, Tetsuya; Koshizuka, Kozo; Williamson, Elizabeth A.; Asou, Hiroya; Said, Jonathan W.; Holden, Stuart; Miyoshi, Isao; Koeffler, H. Phillip
CORPORATE SOURCE: Division of Hematology/Oncology, UCLA School of Medicine, Los Angeles, CA, 90048, USA
SOURCE: Cancer Research (1998), 58(15), 3344-3352
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Troglitazone, a thiazolidinedione derivative, is a widely used antidiabetic drug that binds and activates peroxisome proliferator-activated receptor γ (PPARγ) and enhances insulin sensitivity. It induces differentiation of adipocytes, which highly express PPARγ. We report that human prostate cancer cells expressed PPARγ at prominent levels and normal prostate tissues had very low expression. Dose-response clonogenic assays of the PC-3 prostate cancer cell line with troglitazone showed an antiproliferative effect (ED50, 3 + 10-7 M) and other PPARγ ligands (BRL49653: ED50, 8 + 10-8 M; 15-deoxy-Δ12,14-prostaglandin J2: ED50, 2 + 10-6 M; ciglitazone: ED50, not reached; indomethacin: ED50, not reached) showed similar effects. Combinations of troglitazone and a ligand specific for either retinoid X receptor or retinoic acid receptor did not show a synergistic effect. Pulse-exposure to troglitazone (10-5 M) for different durations showed that 4 days of pulse-exposure to the agent irreversibly inhibited 50% clonal growth of PC-3 cells. Interestingly, PC-3 cells cultured with troglitazone (10-5 M) showed dramatic morphol. changes both by light and electron microscopy, suggesting that the cells became less malignant. Nevertheless, troglitazone did not affect either the cell cycle or several markers of differentiation. LNCaP cells constitutively produced prostate-specific antigen, and levels were markedly enhanced by all-trans-retinoic acid. Troglitazone (10-5 M, 4 days) decreased by 50% the levels of prostate-specific antigen produced by these cells. In vivo treatment of PC-3 tumors growing in male BNX triple immunodeficient mice with oral troglitazone (500 mg/kg/day) produced significant inhibition of

tumor growth (P = 0.01). The only objective side effect of troglitazone in mice was the elevation of serum transaminases. Short-term culture of four surgically obtained human prostate cancer tumors with troglitazone (10-5 M, 4 days) produced marked and selective necrosis of the cancer cells (about 60%) but not the adjacent normal prostate cells. Taken together, these results suggest that troglitazone may be a useful therapeutic agent for the treatment of prostate cancer, especially in the setting of low disease burden.

IT 53-86-1, Indomethacin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ligands for peroxisome proliferator-activated receptor γ demonstrate antitumor effect against human prostate cancer)

RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 43 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:457262 HCAPLUS Full-text
DOCUMENT NUMBER: 129:76495
TITLE: Peripheral benzodiazepine receptor ligands as antiinflammatory agents
INVENTOR(S): McGeer, Patrick L.; Waterfield, J. Douglas; McGeer, Edith G.
PATENT ASSIGNEE(S): Can.
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

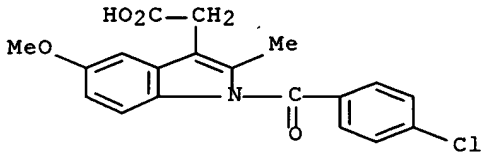
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5776946	A	19980707	US 1995-520211	19950828
CA 2332825	AA	19991202	CA 1998-2332825	19980522
WO 9961024	A1	19991202	WO 1998-CA502	19980522
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9875168	A1	19991213	AU 1998-75168	19980522

EP 1077702 A1 20010228 EP 1998-922551 19980522
R: DE, ES, FR, GB, IT, IE
JP 2002516279 T2 20020604 JP 2000-550484 19980522
PRIORITY APPLN. INFO.: US 1995-520211 A 19950828
WO 1998-CA502 A 19980522

AB Compds. which bind with high affinity to peripheral benzodiazepine receptors are useful as antiinflammatory agents. Such compds. include isoquinoline and benzodiazepine derivs., such as PK 11195. A method of treating an inflammatory condition in a mammal with such compds. is provided. Pharmaceutical compns. comprising such compds. are provided. A method is provided for identifying compds. that are therapeutically effective for treating inflammatory conditions.

IT 53-86-1, Indomethacin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(peripheral benzodiazepine receptor ligands as antiinflammatory agents, and comparisons with other compds.)

RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 44 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:404073 HCAPLUS Full-text
DOCUMENT NUMBER: 129:170177
TITLE: Chemotherapeutic drug-induced apoptosis in human leukemic cells is independent of the Fas (APO-1/CD95) receptor/ligand system
AUTHOR(S): Mcgahon, Anne J.; Pereira, Ana P. Costa; Daly, Lisa; Cotter, Thomas G.
CORPORATE SOURCE: Tumour Biology Laboratory, Department of Biochemistry, University College, Cork, Ire.
SOURCE: British Journal of Haematology (1998), 101(3), 539-547
CODEN: BJHEAL; ISSN: 0007-1048
PUBLISHER: Blackwell Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

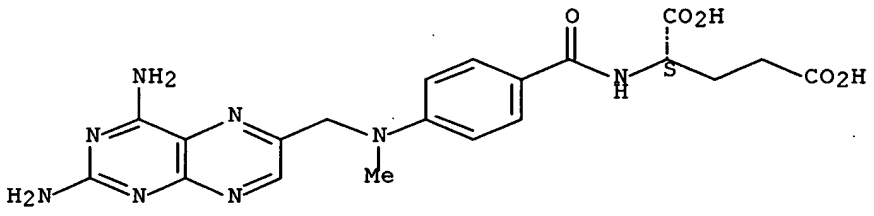
AB The potential role of the Fas (CD95/APO-1) receptor/ligand system in chemotherapeutic drug-induced apoptosis was examined in a number of human leukemic cell lines. Flow cytometric profiles of doxorubicin-treated HL-60, K562, U937 and Jurkat cells failed to show any significant increase in Fas or Fas ligand expression over 24 h, despite the induction of significant levels of apoptosis in these cells. Although preincubation of human leukemic cells with a neutralizing anti-Fas IgG antibody blocked anti-Fas IgM-induced apoptosis, this strategy failed to inhibit chemotherapeutic drug-induced apoptosis. To determine whether recruitment of the Fas/Fas ligand complex during drug-induced apoptosis was a cell-specific event we utilized the CEM

cell line. Doxorubicin treatment of CEM cells over 24 h failed to show any up-regulation in Fas or Fas ligand protein levels as detected by flow cytometry. Furthermore, neutralizing anti-Fas IgG Ab failed to inhibit chemotherapeutic drug-induced apoptosis in CEM cells. The present studies do, however, demonstrate a role for anti-Fas IgM Ab in producing a cytotoxic synergistic effect when used in combination with chemotherapeutic drugs. Low-dose anti-Fas IgM treatment in combination with doxorubicin, methotrexate, camptothecin and etoposide produced an augmented cytotoxicity in CEM cells. Taken together these observations demonstrate that although recruitment of the Fas/APO-1/CD95 receptor/ligand system is not a necessary requirement for chemotherapeutic drug-induced apoptosis, combination of anti-Fas IgM and drug treatment produces a synergistic cytotoxic effect which may prove useful in the treatment of human leukemias.

IT 59-05-2, Methotrexate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(chemotherapeutic drug-induced apoptosis in human leukemic cells is independent of the Fas (APO-1/CD95) receptor/ligand system)

RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

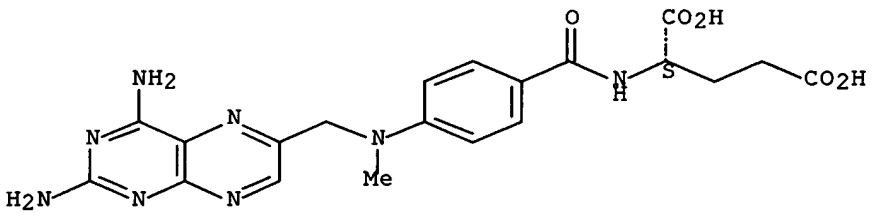


REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 45 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:295496 HCAPLUS Full-text
DOCUMENT NUMBER: 129:80430
TITLE: Effects of cyclosporine A and methotrexate on induction of tumor necrosis factor-alpha and the cell adhesion molecule receptor-ligand pair ICAM-1/LFA-1 in rat cardiac allografts
AUTHOR(S): Ciesielski, Cathleen J.
CORPORATE SOURCE: Loyola Univ., Chicago, IL, USA
SOURCE: (1998) 166 pp. Avail.: UMI, Order No. DA9819597 From: Diss. Abstr. Int., B 1998, 58(12), 6476
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 59-05-2, Methotrexate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(cyclosporine A and methotrexate effects on induction of tumor necrosis factor α and cell adhesion mol. receptor-ligand

pair ICAM-1/LFA-1 in rat cardiac allografts)
RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



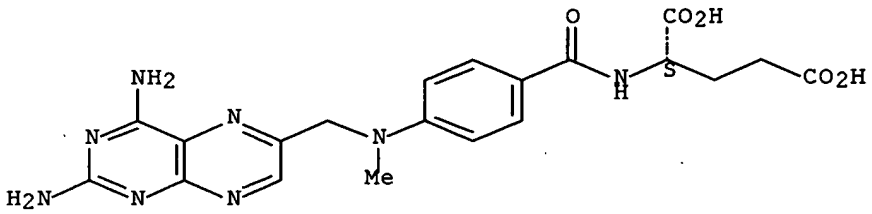
L21 ANSWER 46 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:106734 HCAPLUS Full-text
DOCUMENT NUMBER: 126:194952
TITLE: Drug-induced apoptosis in hepatoma cells is mediated by the CD95 (APO-1/Fas) receptor/ligand system and involves activation of wild-type p53
AUTHOR(S): Mueller, Martina; Strand, Susanne; Hug, Hubert; Heinemann, Eva-Maria; Walczak, Henning; Hofmann, Walter J.; Stremmel, Wolfgang; Krammer, Peter H.; Galle, Peter R.
CORPORATE SOURCE: Department of Internal Medicine IV, Hepatology and Gastroenterology, University Hospital, Heidelberg, 69115, Germany
SOURCE: Journal of Clinical Investigation (1997), 99(3), 403-413
CODEN: JCINAO; ISSN: 0021-9738
PUBLISHER: Rockefeller University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Chemotherapeutic drugs are cytotoxic by induction of apoptosis in drug-sensitive cells. The authors investigated the mechanism of bleomycin-induced cytotoxicity in hepatoma cells. At concns. present in the sera of patients during therapy, bleomycin induced transient accumulation of nuclear wild-type (wt) p53 and upregulated expression of cell surface CD95 (APO-1/Fas) receptor in hepatoma cells carrying wt p53 (HepG2). Bleomycin did not increase CD95 in hepatoma cells with mutated p53 (Huh7) or in hepatoma cells which were p53-/- (Hep3B). In addition, sensitivity towards CD95-mediated apoptosis was also increased in wt p53 pos. HepG2 cells. Microinjection of wt p53 cDNA into HepG2 cells had the same effect. In contrast, bleomycin did not enhance susceptibility towards CD95-mediated apoptosis in Huh7 and in Hep3B cells. Furthermore, bleomycin treatment of HepG2 cells increased CD95 ligand (CD95L) mRNA expression. Most notably, bleomycin-induced apoptosis in HepG2 cells was almost completely inhibited by antibodies which interfere with CD95 receptor/ligand interaction. These data suggest that apoptosis induced by bleomycin is mediated, at least in part, by p53-dependent stimulation of the CD95 receptor/ligand system. The same applies to other anti-cancer drugs such as cisplatin and methotrexate. These data may have major consequences for drug treatment of cancer and the explanation of drug sensitivity and resistance.
IT 59-05-2, Methotrexate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anticancer drug-induced apoptosis in hepatoma cells is mediated by CD95 (APO-1/Fas) receptor/ligand system and involves activation of wild-type p53)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 47 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:628814 HCAPLUS Full-text

DOCUMENT NUMBER: 125:300759

TITLE: New class of potent ligands for the human peripheral cannabinoid receptor

AUTHOR(S): Gallant, Michel; Dufresne, Claude; Gareau, Yves; Guay, Daniel; Leblanc, Yves; Prasit, Petipibbon; Rochette, Chantal; Sawyer, Nicole; Slipetz, Deborah M.; et al.

CORPORATE SOURCE: Merck Frosst Center Therapeutic Research, Dorval, QC, H9R 4P8, Can.

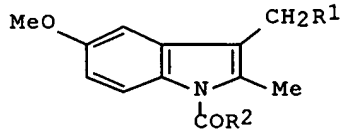
SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(19), 2263-2268
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

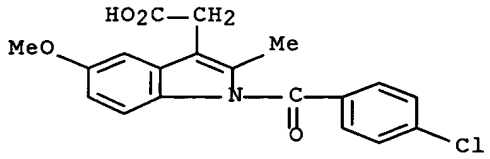
AB Indoles, e.g. I (R1 = morpholino, morpholinocarbonyl, CO2Me, CO2H, morpholinomethyl; R2 = 2-, 4-ClC6H4, 1-, 2-naphthyl, etc.), were prepared as potent ligands for the human peripheral cannabinoid (hCB2) receptor. Two of these indole analogs exhibited nanomolar potencies (Ki) with good selectivity for the hCB2 receptor over the human central cannabinoid (hCB1) receptor.

IT 53-86-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)
(preparation of indoles as ligands for the human peripheral cannabinoid receptor)

RN 53-86-1 HCAPLUS

CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L21 ANSWER 48 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:278215 HCAPLUS Full-text

DOCUMENT NUMBER: 124:331964

TITLE: Involvement of the CD95 (APO-1/Fas) receptor/ligand system in drug-induced apoptosis in leukemia cells

AUTHOR(S): Friesen, Claudia; Herr, Ingrid; Krammer, Peter H.; Debatin, Klaus-Michael

CORPORATE SOURCE: Dep. of Hematology/Oncology, Univ. Children's Hospital, Heidelberg, D-69120, Germany

SOURCE: Nature Medicine (New York) (1996), 2(5), 574-577
CODEN: NAMEFI; ISSN: 1078-8956

PUBLISHER: Nature Publishing Co.

DOCUMENT TYPE: Journal

LANGUAGE: English

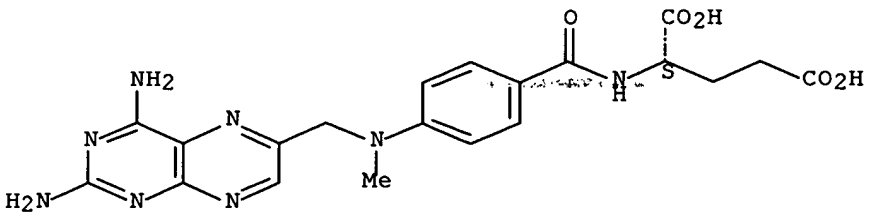
AB Cytotoxic drugs used in chemotherapy of leukemias and solid tumors cause apoptosis in target cells. In lymphoid cells, the CD95 (APO-1/Fas)/CD95 ligand (CD95-L) system is a key regulator of apoptosis. Here the authors describe that doxorubicin induces apoptosis via the CD95/CD95-L system in human leukemia T-cell lines. Doxorubicin-induced apoptosis was completely blocked by inhibition of gene expression and protein synthesis. Also, doxorubicin strongly stimulated CD95-L mRNA expression in vitro at concns. relevant for therapy in vivo. CEM and Jurkat cells resistant to CD95-mediated apoptosis were also resistant to doxorubicin-induced apoptosis. Furthermore, doxorubicin-induced apoptosis was inhibited by blocking F(ab')2 anti-APO-1 (anti-CD95) antibody fragments. Expression of CD95-L mRNA and protein in vitro was also stimulated by other cytotoxic drugs such as methotrexate. The finding that apoptosis caused by anticancer drugs may be mediated via the CD95 system provides a new mol. insight into resistance and sensitivity toward chemotherapy in malignancies.

IT 59-05-2, Methotrexate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(involvement of CD95 (APO-1/Fas) receptor/ligand system in drug-induced apoptosis in human leukemia cells in relation to resistance)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 49 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:896110 HCAPLUS Full-text
DOCUMENT NUMBER: 123:314539
TITLE: Preparation of cytotoxic receptor ligand conjugates linked via lysine radicals.
INVENTOR(S): Lambarde, Victoria K.; Tolman, Richard L.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Brit. UK Pat. Appl., 46 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2282812	A1	19950419	GB 1994-20249	19941007
PRIORITY APPLN. INFO.:			US 1993-138516 A	19931015
OTHER SOURCE(S):	MARPAT 123:314539			

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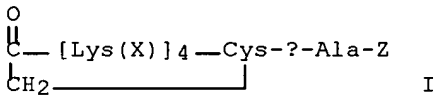


I

AB Cytotoxic receptor ligand scaffolds (CRLS) (Lys)n(Unh)m(Sol)m(X)nZ (Unh = sterically unhindered groups; Sol = hydrophilic, solubilizing groups; n = 3-10; m = 0-5; X = receptor ligand; Z = cytotoxin), were prepared Thus, BrCH2CO-(Lys)4-Cys-β-Ala-OH, prepared by solid phase synthesis on PAM resin, was stirred in aqueous NaHCO3 for 48 h to give cyclic product (I; X = H, Z = OH). This was treated with BrCH2CO2H/DCC to give I (X = COCH2Br, Z = OH), which was coupled to D-Cys6-GnRH in phosphate buffer. The product I (X = COCH2-D-Cys6-GnRH, Z = OH) was coupled with BOC-NHCH2CH2NH2 using BOP/hydroxybenzotriazole followed by deprotection with CF3CO2H/anisole in CH2Cl2 to give I (X = COCH2-D-Cys6-GnRH, Z = NHCH2CH2NH2). This was N-bromoacetylated and conjugated to thiolated exotoxin PE-38M to give a title product contaminated with exotoxin PE-38M. The contaminated product showed a -[log(IC50)] = 8.2 in a competitive binding assay with 125I-buserelin in rat pituitary prepns. The products are claimed for use as chemical sterilants in animals.

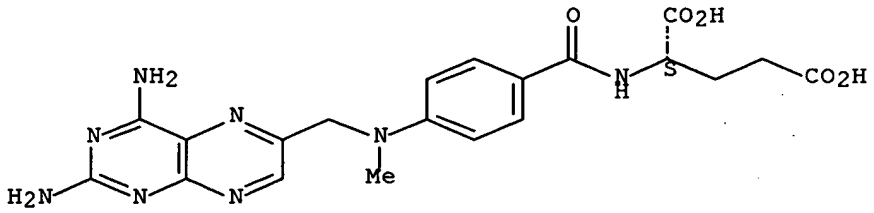
IT 59-05-2DP, Methotrexate, receptor ligand scaffold bound

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cytotoxic receptor ligand conjugates linked via lysine radicals)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 50 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:820336 HCAPLUS Full-text

DOCUMENT NUMBER: 123:222246

TITLE: Flexible ligand docking without parameter adjustment across four ligand-receptor complexes

AUTHOR(S): Clark, Keven P.; Ajay

CORPORATE SOURCE: Dep. Pharmaceutical Chem. & Computer Graphics Lab., Univ. California-San Francisco, San Francisco, CA, 94143, USA

SOURCE: Journal of Computational Chemistry (1995), 16(10), 1210-26
CODEN: JCCHDD; ISSN: 0192-8651

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Understanding mol. recognition is one of the fundamental problems in mol. biol. Computationally, mol. recognition is formulated as a docking problem. Ideally, a mol. docking algorithm should be computationally efficient, provide reasonably thorough search of conformational space, obtain solns. with reasonable consistency, and not require parameter adjustments. With these goals in mind, the author developed DIVALI (Docking wIth eVolutionary ALgorIthms), a program which efficiently and reliably searches for the possible binding modes of a ligand within a fixed receptor. An AMBER-type potential function and search for good ligand conformations using a genetic algorithm (GA) was used. The system was applied to study the docking of both rigid and flexible ligands in 4 different complexes. The results indicated that it is possible to find diverse binding modes, including structures like the crystal structure, all with comparative potential function values. To achieve this, certain modifications to the standard GA recipe are essential.

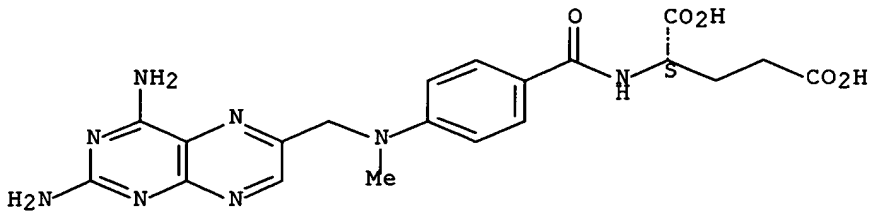
IT 59-05-2D, Methotrexate, dihydrofolate reductase complexes
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(flexible ligand docking without parameter adjustment across 4 ligand-receptor complexes)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzo

yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 51 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:459677 HCAPLUS Full-text
DOCUMENT NUMBER: 122:248300
TITLE: Transferrin receptor specific ligand-neuropharmaceutical agent fusion proteins
INVENTOR(S): Friden, Phillip M.; Starzyk, Ruth M.; Morrison, Sherie L.; Park, Eun-Chung; McGrath, John P.
PATENT ASSIGNEE(S): Alkermes, Inc., USA; Regents of the University of California
SOURCE: PCT Int. Appl., 112 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9502421	A1	19950126	WO 1994-US8000	19940718
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5672683	A	19970930	US 1993-94534	19930716
CA 2166875	AA	19950126	CA 1994-2166875	19940718
AU 9473639	A1	19950213	AU 1994-73639	19940718
AU 693466	B2	19980702		
EP 708661	A1	19960501	EP 1994-922580	19940718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09500381	T2	19970114	JP 1994-504750	19940718

PRIORITY APPLN. INFO.:
US 1993-94534 A 19930716
US 1989-404089 A2 19890907
US 1992-846830 A3 19920306
US 1992-999803 B2 19921120
WO 1994-US8000 W 19940718

AB The present invention pertains to a method for delivering a neuropharmaceutical agent across the blood brain barrier to the brain of a host. The method comprises administering to the host a therapeutically effective amount of a ligand-neuropharmaceutical agent fusion protein wherein the ligand is reactive with a brain capillary endothelial cell receptor. Other aspects of this invention include a delivery system comprising a ligand reactive with a brain capillary endothelial cell receptor which has formed a

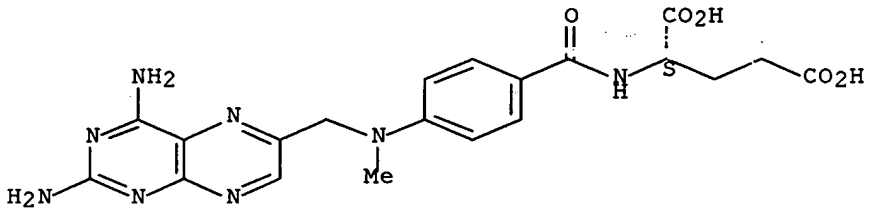
fusion protein with a neuropharmaceutical agent. The fusion proteins are also aspects of this invention.

IT 59-05-2DP, Methotrexate, antibody conjugates
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(transferrin receptor-specific ligand /neuropharmaceutical agent fusion proteins for drug delivery across blood-brain barrier)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 52 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:676029 HCAPLUS Full-text

DOCUMENT NUMBER: 121:276029

TITLE: Evaluating docked complexes with the HINT exponential function and empirical atomic hydrophobicities

AUTHOR(S): Meng, Elaine C.; Kuntz, Irwin D.; Abraham, Donald J.; Kellogg, Glen E.

CORPORATE SOURCE: Sch. Pharmacy, Univ. California, San Francisco, CA, 94143-0446, USA

SOURCE: Journal of Computer-Aided Molecular Design (1994), 8(3), 299-306
CODEN: JCADEQ; ISSN: 0920-654X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Methods that predict geometries of ligands binding to receptor mols. can facilitate ligand discovery and yield information on the factors governing complementarity. The use of atomic hydrophobicities in evaluating binding modes has been examined with four ligand-receptor complexes of known structure. In each system, hundreds of hypothetical binding orientations were generated with DOCK and evaluated using the HINT (Hydropathic INTeractions) exponential function and atomic hydrophobic consts. In three of the four systems, the exptl. binding mode received the best HINT score; in the fourth system, the exptl. binding mode scored only slightly lower than a similar, apparently reasonable orientation. The HINT function may be generally useful as a scoring method in mol. docking.

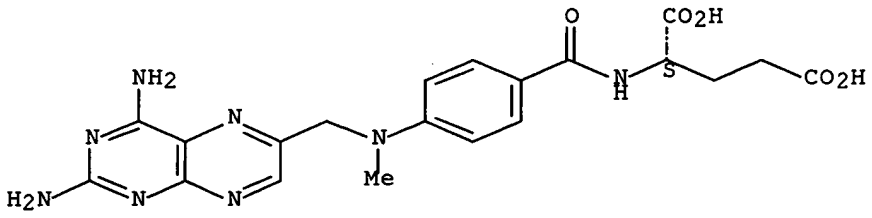
IT 59-05-2, Methotrexate
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(HINT exponential function and atomic hydrophobicities in evaluating binding modes for ligand-receptor complexes)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzo

yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 53 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:417732 HCAPLUS Full-text
DOCUMENT NUMBER: 121:17732
TITLE: Manufacture of melanin cell membrane-specific ligand composition for cosmetic and pharmaceutical use
INVENTOR(S): Redziniak, Gerard; Cerdan, Dominique; Kieda, Claudine; Monsigny, Michel
PATENT ASSIGNEE(S): Parufuan Kurisuchan Deiooru, Japan; Parfums Christian Dior
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06087900	A2	19940329	JP 1992-266381	19921005
JP 3727073	B2	20051214		
US 5332575	A	19940726	US 1992-861780	19920402
US 5686103	A	19971111	US 1996-717976	19960923
PRIORITY APPLN. INFO.:			JP 1991-283587	A1 19911003
			JP 1992-104926	A1 19920423
			US 1992-861780	A3 19920402
			US 1994-221252	B1 19940331

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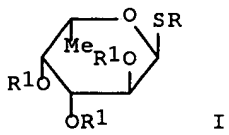


I

AB A compound covalently linked to at least one ligand consisting of an oside residue (particularly fucose, preferably α-L-fucose) capable of approaching to receptors of melanin cells is used for binding a compound to melanin cells by ligand-receptor binding. The said ligand is linked to the compound through a spacer arm such as a hetero-bivalent functional agent or carbohydrate chain

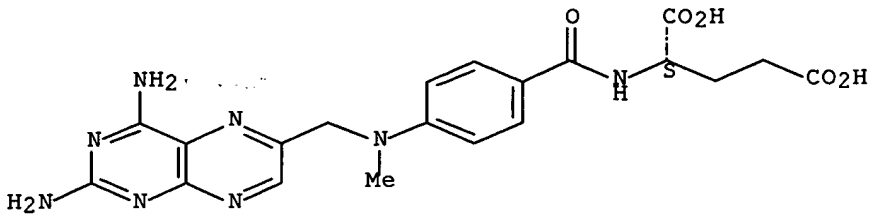
Gal(α1→3)Lac or Gal(1→3)NAc(1→4)Gal(1→4)Glc on the surface of the base structure. The said compound is (1) a natural or synthetic (macro)mol. such as fucolipids (particularly ceramide oligosaccharides having α-L-fucose as the terminus of the carbohydrate chain which are isolated from pig testis or mucus membrane of digestive organs), fucopeptides, fucoproteins (neoglycoproteins, e.g. α-L-fucose-serum albumin conjugate), liposomes, or submicroscopic particles such as polymer nonaparticles or (2) a pharmaceutical and cosmetic substance of dermatol. interest (e.g., an agent for controlling metabolism of melanin cells). A dermatol. composition contains at least one compound described above. A ligand-receptor binding composition consists of a combination of the latter dermatol. composition and a dermatol. or pharmaceutically active substance which act on melanin cells, particularly melanin production function, for skin care or for the treatment of malignant melanin cells or melanoma by promotion or inhibition of melanin production A cosmetic or pharmaceutical composition contains at least one compound described above and cosmetically, pharmaceutically, particularly dermatol. acceptable carriers, vehicles, or additives. Hitherto no sugar receptors on the surface of melanin cells are known, but it was unexpectedly found that fucose residue, particularly α-L-fucose residue is a specific ligand against the melanin cell receptors. This melanin cell membrane-specific ligand composition is effective for regeneration of epidermis and against skin diseases such as lanugo hair and melanin deposition. 2,3,4-Tri-O-acetyl-α-L-fucopyranosyl bromide and thiourea were refluxed in acetone for 3 h under N to give 2-S-(2,3,4,-tri-O-acetyl-α-L-fucopyranosyl)-2-thiopseudourea hydrobromide [I; R = C(:NH)NH2.HBr, R1 = Ac] which was reacted with 3-iodopropionic acid in the presence of Na2CO3 and Na2S2O5 in aqueous acetone followed by deacetylation with MeOH containing Et3N and H2O to give thiofucoside I (R = CH2CH2CO2H, R1 = H). The latter compound was dissolved in H2O which was adjusted to pH 5.5 with HCl and condensed with 1,3-diamino-2-hydroxypropane by using 1-ethyl-3-(3- dimethylaminopropyl)carbodiimide to give I.HCl [R = CH2CH2CONHCH2CH(OH)CH2NH2, R1 = H] which was acylated by succinimidyl S-acetylthioacetate in DMF containing Et3N followed by deacetylation with aqueous EDTA containing excess HONH2 to give I [R = CH2CH2CONHCH2CH(OH)CH2NHCOCH2SH, R1 = H], which is used in liposomes. A sun screen cream was obtained by mixing (1) an emulsion containing perhydrosqualene 39.2, soya lecithin o.8, and distilled H2O 220.0 g and (2) a liposome gelatinized suspension liquid comprising (A) lipid phase component containing dipalmitoylphosphatidylcholine 0.48, cholesterol 0.26, dicetyl phsophate 0.09, fucosylated dipalmitoylphosphatidylethanolamine (preparation from p-isocyanatophenyl α-L-fucopyranoside and dipalmitoylphosphatidylethanolamine given) 0.16, and forskolin 0.01 g, (B) 1 g aqueous phase component (hydratable coleus extract), (C) 1 g gel-like additive (neutralized carbopol 940), and (D) 100 g distilled H2O, fragrant material, UV filter, and preservative.

IT 59-05-2, Methotrexate
RL: BIOL (Biological study)
(ligand-receptor binding pharmaceutical composition containing melanin cell membrane-specific fucose-containing ligand and, for treatment of melanoma)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



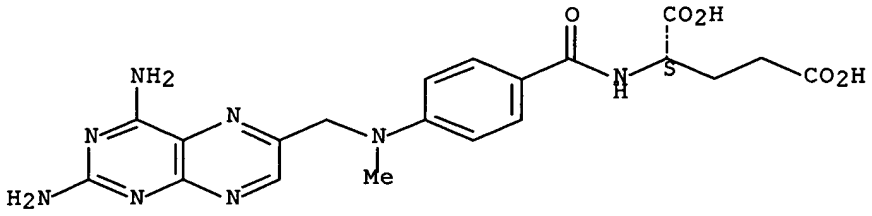
L21 ANSWER 54 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:62317 HCAPLUS Full-text
DOCUMENT NUMBER: 120:62317
TITLE: Delivery of a cytotoxic compound to a cancer cell using a pathway of plasminogen activator material
INVENTOR(S): Jankun, Jerzy; Hart, Richard
PATENT ASSIGNEE(S): University of Toledo, USA
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9324141	A1	19931209	WO 1993-US5034	19930527
W: AU, BR, CA, JP, NO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9343942	A1	19931230	AU 1993-43942	19930527
EP 643584	A1	19950322	EP 1993-914191	19930527
EP 643584	B1	20000315		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AT 190501	E	20000415	AT 1993-914191	19930527
ES 2143504	T3	20000516	ES 1993-914191	19930527
US 5679350	A	19971021	US 1996-646561	19960508
PRIORITY APPLN. INFO.:			US 1992-889783 A	19920528
			US 1993-59813 A	19930510
			WO 1993-US5034 A	19930527
			US 1994-294950 B1	19940824

AB A cytotoxic compound is delivered into a cancer cell by coupling it to a plasminogen material such as a plasminogen activator inhibitor (PAI-1) which binds to urokinase plasminogen activator (uPA). The uPA is bound to the cell surface by uPA receptors, and the resultant complex is internalized to deliver the cytotoxic compound within the cell. Thus, a conjugate of PAI-1 with cholera toxin A chain was labeled with TRITC and bound to colloidal Au particles. When the particles were incubated with HT1080 fibrosarcoma cells expressing very low amts. of receptor-bound uPA, binding of the particles to the cell surface was revealed by SEM, and internalization of the PAI-1-toxin conjugate was demonstrated by fluorescence microscopy.

IT 59-05-2D, Methotrexate, conjugates with plasminogen activator ligands
RL: BIOL (Biological study)
(for targeting to urokinase-receptor complex on neoplasm cell surface)
RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L21 ANSWER 55 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:19660 HCAPLUS Full-text
DOCUMENT NUMBER: 116:19060
TITLE: Chimeric antibodies with receptor-binding ligands in place of their constant region
INVENTOR(S): Morrison, Sherie L.; Shin, Seung Uon
PATENT ASSIGNEE(S): Columbia University, USA
SOURCE: PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9114438	A1	19911003	WO 1991-US1844	19910320
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
CA 2078689	AA	19910921	CA 1991-2078689	19910320
CA 2078689	C	20030211		
AU 9175582	A1	19911021	AU 1991-75582	19910320
AU 654811	B2	19941124		
EP 521985	A1	19930113	EP 1991-906955	19910320
EP 521985	B1	19970924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 05506574	T2	19930930	JP 1991-507276	19910320
JP 3319594	B2	20020903		
AT 158615	E	19971015	AT 1991-906955	19910320
PRIORITY APPLN. INFO.:			US 1990-496409 A2	19900320
			WO 1991-US1844 A	19910320

AB A modified chimeric monoclonal antibody (MAb) comprises 2 shorter polypeptides functioning as the light chains of the Ab and 2 longer polypeptides functioning as heavy chains. The longer chains have a variable region characteristic of a 1st mammal and a constant region characteristic of a 2nd mammal; at least a portion of the constant region is replaced with a receptor-binding ligand. Immunol. reactive complexes and chimeric polypeptides are also disclosed, as are recombinant methods of producing chimeric MAbs, immunol. reactive complexes, and chimeric polypeptides. The MAbs are useful in pharmaceuticals for delivering drugs (e.g. in treatment of neoplasms) and in detecting cells having a receptor targeted by the ligand at the constant region of the MAb. The cDNA encoding the VH, CH1, hinge, and 1st amino acid of CH2 from a chimeric mouse/human IgG3 anti-dansyl antibody was joined to a cDNA encoding rat insulin-like growth factor 1 (IGF1) immediately 3' to the leader sequence of IGF1. The chimeric heavy chain gene vector and a vector

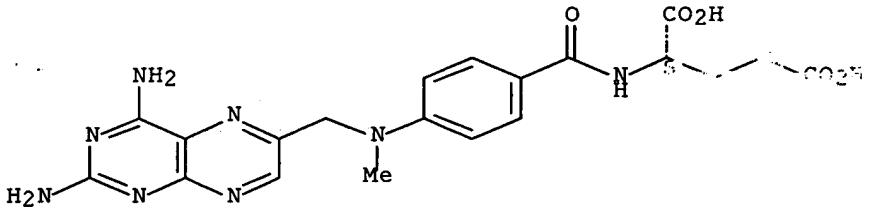
encoding an anti-dansyl chimeric K light chain were introduced into myeloma P3X63Ag8.653. The chimeric IgG3-protein was produced and secreted at 30 μg/106 cells/24h, had specificity for the dansyl antigen, and bound the IGF1 receptors of human lymphoblast IM-9. The activity and binding was similar but reduced compared with human IGF1.

IT 59-05-2D, Methotrexate, chimeric monoclonal antibody conjugates
RL: PRP (Properties)
(receptor-binding ligand in heavy chain of)

RN 59-05-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



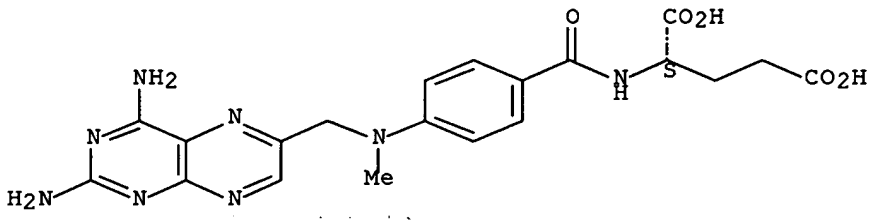
L21 ANSWER 56 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:523446 HCAPLUS Full-text
DOCUMENT NUMBER: 97:123446
TITLE: Determination of ligands or receptors by means of competition reaction. Test kit for carrying out the process and its application
INVENTOR(S): Thoma, Hans A.
PATENT ASSIGNEE(S): Fed. Rep. Ger.
SOURCE: Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 55868	A2	19820714	EP 1981-110852	19811230
EP 55868	A3	19820804		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DE 3100061	A1	19820805	DE 1981-3100061	19810102
JP 57132898	A2	19820817	JP 1981-215976	19811228
PRIORITY APPLN. INFO.:			DE 1981-3100061 A	19810102

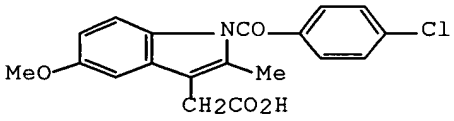
AB Ligands or receptors are determined by an immunoassay which uses a conjugate of a label with a binding component A (e.g., an antibody) as well as a specific binding component B (e.g., another antibody), which binds the label in the unreacted label-binding component A conjugate. The free binding sites on binding component B are saturated with label, and the amount of free label is determined with a signal mol. In 1 example, testosterone was determined with methotrexate-antitestosterone antibody conjugate, testosterone-IgG conjugate, antimethotrexate antibody, and methotrexate. Determination of free methotrexate was performed with dihydrofolate reductase and NADPH. Other examples include detns. of IgG and testosterone-binding globulin.

IT 59-05-2
RL: ANST (Analytical study)
(in immunoassays for ligands or receptors)
RN 59-05-2 HCAPLUS
CN L-Glutamic acid, N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



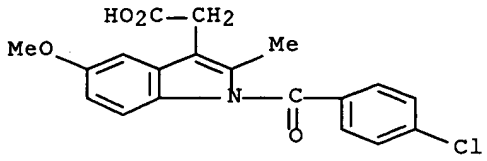
L21 ANSWER 57 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:25075 HCAPLUS Full-text
DOCUMENT NUMBER: 94:25075
TITLE: Effect of indomethacin on cardiac β-adrenergic receptors
AUTHOR(S): Feuerstein, Giora; Torda, Tichomir; Kopin, Irwin J.
CORPORATE SOURCE: Lab. Clin. Sci., Natl. Inst. Ment. Health, Bethesda, MD, 20205, USA
SOURCE: European Journal of Pharmacology (1980), 67(4), 469-72
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



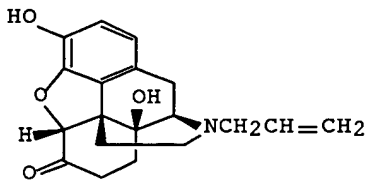
I

AB Treatment of rats with indomethacin (I) [53-86-1], 1.5 mg/kg/day, for 1 wk, decreased the number of β-adrenoceptors in the heart without altering their affinity for the specific β-adrenergic ligand. In indomethacin-treated rats, there was a reduction in the cardiac response to epinephrine [51-43-4] in vivo as indicated by a shift to the right of the epinephrine dose-heart response curve. These results support a possible interference by indomethacin in β-adrenoceptor- mediated effects.

IT 53-86-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(β-adrenergic receptor of heart response to)
RN 53-86-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L21 ANSWER 58 OF 58 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:180140 HCAPLUS Full-text
DOCUMENT NUMBER: 90:180140
TITLE: Facilitatory effect of naloxone and involvement of specific ligand-opiate receptor system in the antinociceptive effects of non-opioid drugs
AUTHOR(S): Ramabadran, K.; Jacob, J. J. C.
CORPORATE SOURCE: Lab. Pharmacol., Pasteur Inst., Paris, Fr.
SOURCE: Archives Internationales de Pharmacodynamie et de Therapie (1978), 236(1), 27-42
CODEN: AIPTAK; ISSN: 0003-9780
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The facilitatory effects exerted by naloxone-HCl (I-HCl) [357-08-4] on a nociceptive reaction (jumping) in the hot plate test was not modified by 3 phosphodiesterase inhibitors, theophylline, Ro-20-1724 and I.C.I 63197 which themselves had different effects on the latency of jumping. The facilitatory effects of naloxone were not diminished by neuroleptics,, cholinergic agonists, or miscellaneous drugs (baclofen [1134-47-0], indomethacin [53-86-1], ketoprofen [22071-15-4], n-dipropylacetate [99-66-1], diazepam [439-14-5], and K chlorazepate [57109-90-7]). I antagonized the antinociceptive effects of neuroleptics in different patterns. No competitive component could be observed with haloperidol [52-86-8], whereas such a phenomenon was apparent with benperidol [2062-84-2]. Pimozide [2062-78-4] was an intermediary case. The antinociceptive effects of 2 cholinergic agonists, arecoline-HBr [300-08-3] and eserine salicylate [57-64-7] were antagonized by I and stereospecifically by the (-) isomer, Mr 2266 [56649-76-4]. The (+) isomer, Mr 2267 [56649-75-3] was inactive. The antagonism by the opioid antagonists of the antinociceptive effects of cholinergic agonists appeared to be of a competitive type. Thus, the facilitatory effects of I did not apparently involve activation of adenyl cyclase [9012-42-4] or the mediation of dopaminergic or cholinergic (neural) structures. The antinociceptive effects of benperidol and pimozide but not of haloperidol might result from the

triggering of specific opiate receptors and those of cholinergic agonists from such a triggering and/or from release of endogenous ligands.

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